CREATING ORIGEN MODELS

THESIS

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THESIS

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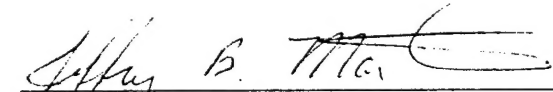Captain, USA

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Abstract

The purpose of this study was to develop a methodology for creating problem-dependent cross section libraries for ORIGEN (Oak Ridge Isotope Generation and Depletion Code). The Air Force Technical Applications Center (AFTAC) has a requirement to classify spent nuclear fuel. The ORIGEN codes provide generic models of commercial nuclear reactor designs that are not adequate for the detailed analysis required by AFTAC. After comparing the methods that ORIGEN2 and ORIGEN-S use to develop burnup-dependent cross section libraries, the research focused on developing a methodology for creating new ORIGEN-S models. Models of the Ohio State University Research Reactor were created using the Coupled 1-D Shielding Analysis (SAS2H) module of the Modular Code System for Performing Standardized Computer Analysis for Licensing Evaluation (SCALE4.3). Model design parameters were examined by varying the fuel loading, composition temperatures, larger unit cells, and power histories. The results indicate that the SAS2H sequence has the potential to fulfill the technical requirements of the sponsor.

CREATING ORIGEN MODELS

I. Introduction

Background

The Air Force Technical Applications Center (AFTAC) monitors
compliance with several nuclear treaties. It is the sole DOD agency that
operates a global network of sensors and laboratories that provide national
authorities technical measurements to monitor foreign nuclear activity
(AFTAC, 1997). It also conducts research and development of proliferation
detection technologies for all weapons of mass destruction. One of the
challenges facing AFTAC is distinguishing between spent nuclear reactor fuel
and material created during a nuclear test. Modeling of nuclear reactors and
their fuel cycles using the Oak Ridge Isotope Generation and Depletion Code
(ORIGEN) will enhance AFTAC's ability to characterize spent nuclear fuel.

ORIGEN is a computer code that computes time-dependent
concentrations and source terms of a large number of isotopes, which are
simultaneously generated and depleted through neutronic transmutation,
fission, radioactive decay, input feed rates, and physical or chemical removal
rates (Hermann and Westfall, 1997:F7.iii). The code estimates nuclear fuel

composition after irradiation. This information is useful when analyzing the spent fuel.

Problem Statement

The purpose of this thesis is to develop a methodology for creating models for ORIGEN and demonstrate it by modeling the Ohio State University Research Reactor (OSURR). The objective of the thesis is to determine what raw data is required, and develop a technique to transform the data into the input libraries used by ORIGEN.

Scope

This thesis describes the process of creating models for the ORIGEN2 and ORIGEN-S codes. A sample case using the OSURR was performed using ORIGEN-S. The effects of model unit cells, temperature, and reactor power history were studied by modifying the input parameters in the code's input files.

Assumptions

- The Light Water Reactor ENDF cross section libraries supplied with the SCALE4.3 code are applicable to the research reactor.

- Many of the computer codes that were used are based on simplifying assumptions that are discussed in Chapters II through IV.

General Approach

The problem can be divided into five tasks:

    1)   Organize the theory of ORIGEN to identify the code's assumptions and limitations, tasks, and software to do the tasks

2)   Develop the computer module procedure to build an ORIGEN cross-section library.

3)   Identify and collect the design data required to model the OSU Research Reactor.

4)   Build a cross-section library and input file set to model the OSU Research Reactor fuel cycle.

5)   Perform parameter studies to demonstrate the use of the code and to evaluate the sensitivity of the results to the approximations made in modeling the core.

Organization

Chapter II describes ORIGEN and its analytical method, compares the different versions of the code, and provides the results of validation studies of the code. Chapter III compares the methods used to prepare new models for two different versions of the code: ORIGEN2 and ORIGEN-S. Chapter IV then explains why ORIGEN-S was selected for this research and provides details about the code modules that prepare cross sections. Chapter V describes the methodology used to create a model of the Ohio State Research Reactor. The results of design parameter studies are presented in Chapters VI and VII. Chapter VIII presents the conclusions and recommendations derived from the research.

II. Description of ORIGEN

History (Ludwig and Renier, 1989:1-3)

The Chemical Technology Division at Oak Ridge National Laboratory (ORNL) developed the ORIGEN computer code. The code was principally intended for use in estimating spent fuel and waste characteristics for the design and study of fuel reprocessing plants, shipping casks, and waste treatment and disposal facilities. The initial version, released in 1973, modeled four common reactor types: HTGR, LWR, LMFBR, and MSBR. The Radiation Safety Information Computational Center (RSICC) at ORNL made ORIGEN available worldwide. Many organizations adopted ORIGEN because of its simplicity and convenient detailed output. The uses of ORIGEN shifted from generic fuel cycle applications to specific calculations for environmental impact studies. With the release of ORIGEN2 in 1980, ORIGEN and its associated databases were expanded to include specific LWR and BWR types with various fuel cycles. Versions of the code were also developed for a variety of computing platforms, including the PC. Currently, ORIGEN can be found in five different forms: ORIGEN2.1, ORIGEN-ARP, ORIGEN-JR, ORIGEN-S, and a variant developed in Germany, ORIGEN-JUEL-II.

Analytical Method

ORIGEN is a FORTRAN code package that determines the isotopic composition of a fuel sample after irradiation. ORIGEN uses a matrix exponential method to solve a system of nonhomogeneous, first-order, ordinary differential equations of the form:

$$\frac{dX_i}{dt} = \sum_{j=1}^{N} l_{ij} \lambda_j X_j + \phi \sum_{k=1}^{N} f_{ik} \sigma_k X_k - (\lambda_i + \phi \sigma_i + r_i) X_i + F_i \tag{1}$$

where

$X_i =$ atom density of nuclide i,

$N =$ number of nuclides,

$l_{ij} =$ fraction of radioactive disintegration by other nuclide j which leads to formation of nuclide i,

$\lambda_i =$ radioactive decay constant for nuclide i,

$\phi =$ position and energy-averaged neutron flux,

$f_{ik} =$ fraction of neutron absorption by other nuclide k which leads to formation of nuclide i,

$\sigma_k =$ spectrum-averaged neutron absorption cross section of nuclide k,

$r_i =$ continuous fractional removal rate of nuclide i from the system,

$F_i =$ continuous feed rate of nuclide i.

ORIGEN assumes that the space-energy-averaged flux can be considered constant over time steps Δt. Similarly, ORIGEN assumes that a single set of flux-weighted neutron cross sections is adequate for use over a time step. These assumptions are required to consider Equation (1) as a first-order, linear differential equation (Hermann and Westfall, 1997:F7.2.1).

Equation (1) can be written using vector notation:

$$\dot{x} = \Lambda x + \phi \Sigma x + f, \tag{2}$$

where

$$\Lambda = (l_{ij} - \delta_{ij})\lambda_j - \delta_{ij}r_j,$$
$$\Sigma = f_{ij}o_j - \delta_{ij}o_j, \text{ and}$$
$\mathsf{x} = $ vector of nuclide atom densities
$\mathsf{f} = $ vector of nuclide feed rates.

A coefficient matrix, A, is creating by combining terms,

$$\mathsf{A} = \Lambda + \phi\Sigma. \tag{3}$$

After substitution an equivalent form of Equation (2) is expressed as

$$\dot{\mathsf{x}} = \mathsf{A}\mathsf{x} + \mathsf{f}. \tag{4}$$

ORIGEN can consider 1700 nuclides, which in turn produces a 1700 by 1700 coefficient matrix. The typical nuclide has fewer than 12 parents making the coefficient matrix very sparse. ORIGEN makes use of indexing techniques that store only nonzero elements in order to reduce storage requirements. The transition matrix (an array of transformation rates of each parent to daughter nuclide) is efficiently stored in this way.

ORIGEN calculates the neutron flux using the following equation:

$$\phi = \frac{CP}{\sum_i X_i^f \sigma_i^f R_i} \tag{5}$$

where

$\phi = $ instantaneous neutron flux (n cm^{-2} s^{-1}),

$C = \;\; 1.037 \times 10^{19} \dfrac{\mathrm{b \cdot (g\ atom) \cdot eV \cdot n}}{\mathrm{cm^2 \cdot J \cdot fission}}$,

$P = $ power (MW),

$X_i^f = $ amount of fissile nuclide i in fuel (g atom),

$\sigma_i^f = $ microscopic fission cross section for nuclide i (b),

$R_i =$ recoverable energy per fission for nuclide i (MeV/fission).

Equation (5) calculates the neutron flux at the beginning of a discrete time step rather than the average neutron flux of the time step. ORIGEN expands Equation (5) in a Taylor series through second-order terms with X_i^f as the time-dependent variables (Croff, 1983:341). The average neutron flux is then calculated by integrating the expansion over the time step and dividing by the length of the time step. The neutron-induced transformation rate coefficients, $f_{ik} \, \sigma_k$ and σ_i, in the transition matrix are multiplied by the ratio of the average neutron flux for the current time step to the average neutron flux for the previous time step to adjust them to the correct flux for the current time step.

ORIGEN data libraries include cross sections for three neutron energy ranges: thermal (below 0.5 eV), a resonance energy range extending to 1 MeV, and a fast energy range above 1 MeV. Three factors, THERM, RES, and FAST, are used to weight the cross sections with the neutron flux. THERM is used to adjust the 2200-m/s cross section in the library for a thermal neutron spectrum corresponding to a known value of reactor moderator temperature. RES and FAST are used to weight the other cross sections relative to the thermal cross sections in forming one-group values (Hermann and Westfall, 1997: F7.2.10).

The neutron flux is derived from the power level using one-group cross sections, and then the system of simultaneous differential equations is solved

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through a composite of solution methods. The solution of the system of equations contains terms of the form, $e^{\lambda t}$, where λ is a negative number. These terms decay to zero as t increases, but numerical approximations generally will not have this property unless restrictions are placed on the size of the time step. This problem is particularly acute when a solution consists of a steady-state term that is coupled with a transient term that decays rapidly to zero, causing the error associated with the decaying transient to dominate the calculations and produce meaningless results (Burden and Faires, 1993:314). The variation in the magnitudes of the transition rate coefficients results in a stiff system of equations. Nuclides with large rate constants are removed from the transition matrix using a relation based on the norm of the matrix and the duration of the time step in order to avoid the problems associated with the stiffness of the system. A set of asymptotic solutions is used to handle the buildup and decay of short-lived nuclides that do not have long-lived precursors. These nuclides approach a constant concentration within the time step. The Gauss-Seidel iterative technique is used for short-lived nuclides that have long-lived precursors, by assuming that the short-lived daughter and subsequent short-lived progeny are in secular equilibrium with their parents (Hermann and Westfall, 1997:F7.2.6).

The next solution method uses the matrix exponential method to deal with the long-lived nuclides. Eliminating the short-lived nuclides creates a

reduced transition matrix. Without a continuous feed this matrix is a system of homogenous equations:

$$\dot{x}(t) = Ax(t) \tag{6}$$

where

$\dot{x}(t) =$ time derivative of the nuclide concentrations,
$A =$ reduced transition matrix containing transformation rate constants, A is assumed to be constant during a time step, and
$x(t) =$ nuclide concentrations.

Equation (6) has the solution:

$$x = \exp(At)x_0 \tag{7}$$

where

$x =$ concentration of each nuclide at time t,
$x_0 =$ vector of initial nuclide concentrations, and
$t =$ time at end of each time step.

The exponential in Equation (7) can be expanded in a series expansion as:

$$\exp(At) = I + At + \frac{(At)^2}{2} + \ldots = \sum_{m=0}^{\infty} \frac{(At)^m}{m!} \tag{8}$$

Where I represents the identity matrix. After substitution Equation (7) becomes:

$$x = \left[I + At + \frac{(At)^2}{2!} + \frac{(At)^3}{3!} + \ldots \right] x_0 \tag{9}$$

Equation (9) is a series of terms that arise from the successive post-multiplication of the transition matrix by the vector of nuclide concentration increments produced from the computation of the previous terms.

$$x = x_0 + tAx_0 + \frac{t}{2}A(tAx_0) + \frac{t}{3}A\left[\frac{t}{2}A(tAx_0)\right] + \cdots \tag{10}$$

A recursion relationship is developed from Equation (10) by defining the vectors c_n as

$$c_0 \equiv x_0, \ c_{n+1} = \frac{t}{n+1}Ac_n,$$

yielding a solution of the form:

$$x = \sum_{n}^{\infty} c_n. \tag{11}$$

The solution for the system of nuclides given in Equation (11) then only requires the storage of three vectors, c_n and c_{n+1}, in addition to the current value of the solution x_0 (Hermann and Westfall, 1997:F7.2.3). A relation using the matrix norm determines the number of terms required to limit the summation error in Equation (11) to less than 0.1% (Hermann and Westfall, 1997:F7.2.4).

The solution for the nonhomogeneous case, $\dot{x} = Ax + f$, is

$$x = e^{At}x_0 + \left[e^{At} - I\right]A^{-1}f. \tag{12}$$

The exponentials in Equation (12) are expanded in a series expansion yielding a solution for a system of m nuclides that is the sum of the homogeneous and particular solutions,

$$\mathbf{x} = \sum_{m=0}^{\infty} \frac{(At)^m}{m!} \mathbf{x}_0 + \sum_{m=0}^{\infty} \frac{(At)^m}{(m+1)!} \mathbf{f}t .$$

(13)

A second recursion relationship for the particular solution, $\mathbf{x}^P$, is developed by defining the vectors $\mathbf{d}_n$ as,

$$\mathbf{d}_1 \equiv \mathbf{f}t , \quad \mathbf{d}_{n+1} = \frac{t}{n+1} A \mathbf{d}_n .$$

Yielding a solution

$$\mathbf{x}^P = \sum_{n=1}^{\infty} \mathbf{d}_n .$$

(14)

The solution for the nonhomogeneous case then can be written as,

$$\mathbf{x} = \sum_{n=0}^{\infty} \mathbf{c}_n + \sum_{n=1}^{\infty} \mathbf{d}_n .$$

(15)

Comparison of Codes

ORIGEN2.1 is the current version of the original code. ORIGEN-JR is a less robust version that is capable of handling 850 nuclides compared to the 1700 considered by ORIGEN2.1. The German variant, ORIGEN-JUEL-II, can make use of irradiation-histogram data of fuel batches given in the form of multigroup cross section and multigroup neutron fluxes, both varying with time during the irradiation period of the fuel.

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ORIGEN-S was designed to be the point depletion module of SCALE (Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation for Workstations and Personal Computers). Although capable of stand-alone operation, ORIGEN-S was designed to interface with the other neutronic modules of SCALE to obtain and use problem-dependent cross section libraries for each analysis (Parks, 1992:57-58). ORIGEN-S uses the same matrix exponential technique as ORIGEN2.1, but differs in the methodology used to prepare and provide the neutronic data for the code. Due to the modular nature of the SCALE system, the input format of ORIGEN-S is incompatible with ORIGEN2.1.

Point-depletion codes like ORIGEN2.1 and ORIGEN-S solve for nuclide concentrations using cross section data and spectrum parameters averaged over the spatial region of interest. All of the spatial influences (core geometry, moderator density, enrichment variation) that affect the prediction of nuclide isotopics must be incorporated into the averaged cross section and spectrum data applied to the codes as a function of burnup. The difference in methods used to develop and supply the burnup-dependent cross section libraries is the primary difference between ORIGEN2.1 and ORIGEN-S (Parks, 1992:59).

One of the advantages of the ORIGEN system is the variability of actinide cross sections among time steps. There are two reasons why constant average cross sections generate incorrect depletion results:

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1)   the cross sections of some isotopes do not vary linearly with burnup,

2)   the cross sections near the end of an irradiation cycle are more important in determining spent fuel composition than the cross sections at the beginning of the cycle.

The use of burnup dependent cross sections addresses these issues (Ludwig and Renier, 1989:29).

ORIGEN2.1 uses cross section and fission product yield libraries that have been developed for specific reactor models. A model is defined as a specific reactor design with a specified fuel cycle. The cross section libraries provided with the original ORIGEN code were computed using simplified, one-dimensional, multi-energy-group reactor physics calculations. When the cross section libraries were updated for ORIGEN2, more sophisticated, multidimensional computations were used. While more computationally intensive, the use of multidimensional computations allows important spatial variations (axial variation of moderator density, pin-to-pin fuel enrichment, boron moderator concentration) to be incorporated explicitly in the neutronic analysis (Parks, 1992:59).

An ORIGEN2.1 cross section library consists of one-energy-group cross sections at varying burnups for a specific reactor model. ORIGEN2.1 estimates the average nuclear material burnup for each irradiation time step and obtains the appropriate actinide cross sections by interpolation. These

interpolated cross sections are then substituted into the transition matrix (Parks, 1992:61).

ORIGEN-S relies on other SCALE modules to compute burnup dependent cross sections rather than requiring a pre-calculated problem dependent library. At each time step, the SAS2H module sequence performs a radiation transport analysis to obtain cross sections and spectrum parameters for the ORIGEN-S point depletion analysis (Parks, 1992:59). While more flexible than the ORIGEN2.1 method, the calculations performed by the SCALE modules are one-dimensional computations and produce *assembly-averaged* fluxes which do not model the spatial variations as rigorously as the multidimensional calculations used to generate the ORIGEN2.1 libraries.

An automatic rapid processing (ARP) methodology has been developed for use with ORIGEN-S in order to speed up calculations. This method uses an interpolation scheme, similar to the ORIGEN2.1 method, rather than performing a transport analysis at each time step in order to obtain burnup dependent cross sections. The ARP methodology interpolates cross sections using fuel enrichment and burnup as the independent variables. The SAS2H module sequence is used to create a cross section library as a function of burnup and enrichment from which the interpolations are performed (Leal, Hermann, and Parks, 1995:52-52).

<u>Validation Studies</u>

Although the example models developed for this research could not be validated by conducting an isotopic analysis of the spent fuel, the use of ORIGEN to predict spent fuel has been validated in other research, described below.

ORIGEN-S was used to predict the isotopic composition of CANDU UO_2 fuel. The measured inventories of several isotopes (^{235}U, ^{236}U, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{244}Cm) agreed to within 5%, with others varying by up to 20% (^{234}U, ^{238}Pu, ^{237}Np). The major fission products (^{134}Cs, ^{137}Cs, ^{90}Sr) were predicted to within 3% of the measured values (Tait, Gauld, and Kerr, 1994:119).

The Chemical Technology Division of ORNL conducted a study on the spent fuel from the H. B. Robinson, Oconee-1, and Turkey Point-3 reactors using an unspecified version of ORIGEN. Isotopes were grouped into three categories based on agreement between calculated predictions and experimental data. The results are presented in Table II-1 (Mailen and Roddy, 1987:577).

Table II-1: Relative Agreement of Experimental Data and ORIGEN Predictions

Excellent (within ± 10%)	Fair (within ± 50%)	Poor (>50%)
^{234}U	^{238}Pu	^{79}Se
^{235}U	^{242}Pu	^{126}Sn
^{236}U	^{242}Cm	^{154}Eu
^{237}Np	^{245}Cm	
^{239}Pu	^{3}H	
^{240}Pu	^{85}Kr	
^{241}Pu	^{99}Tc	
^{241}Am	^{129}I	
^{242}Am	^{125}Sb	
^{243}Am	^{134}Cs	
^{244}Cm	^{144}Ce	
^{246}Cm		
^{247}Cm		
^{14}C		
^{90}Sr		
^{106}Ru		
^{137}Cs		

A similar study that was performed on spent fuel from the Calvert Cliffs-1 and Obrigheim reactors using SAS2H/ORIGEN-S focused on 27 nuclides of interest. The calculated values were in close agreement with the measured values (22 nuclides agree within 10%, 5 within 20.2%) (Hermann, Brady, and Parks, 1991:147-149).

These validation and verification activities indicate that the methodology used by the ORIGEN codes is reliable. They also show that the accuracy of the codes is dependent on the quality of the decay, photon production, fission yield, and cross section data (Parks,1992:63).

III. Method

Introduction

This chapter describes the methodology involved in developing new models for ORIGEN. As described in the previous chapter, ORIGEN requires cross section and flux parameters in order to perform depletion calculations. The next section describes the process used to develop a new cross section library for ORIGEN2. The last section describes the use of the SAS2H module of SCALE to create new models using ORIGEN-S.

ORIGEN2

S. B. Ludwig and J. P. Renier of ORNL created extended-burnup models for PWR and BWR reactors during the late 1980's, using 15 different computer modules to create new ORIGEN cross section libraries. Their technique transformed generic cross section data into a new problem dependent ORIGEN cross section library. The first step is to create an 84-energy group master library that consists of two classes of actinides: resonance and nonresonance. The second step is to perform fuel-cell neutron energy spectrum calculations at different burnups to account for self-shielding effects of the nuclides in the core. This step transforms the 84-energy group library into few-group (12 and 4 energy groups) libraries. The third step is to perform fuel depletion calculations using the few-group, self-shielded cross sections to produce a one-group, burnup dependent cross

section for the most neutronically important actinides. The fourth step determines the multigroup neutron energy spectrum by performing reactor physics calculations for the specific reactor/fuel problem. This spectrum is then used to weight the multigroup cross sections to prepare a master, one-group cross section library and calculate the ORIGEN flux parameters. The fifth and final step is to convert the AMPX format library into an ORIGEN readable input library (Ludwig and Renier, 1989:27-28).

ORIGEN-S

Overview. A review of current computer codes available through the Radiation Safety Information Computational Center (RSICC) identified SCALE as a potential candidate for developing new ORIGEN models. SAS2H: A Coupled One-Dimensional Depletion and Shielding Analysis Module is part of the SCALE 4.3 system. The module was originally developed to generate radiation source terms for the shielding analysis of shipping casks. The module is principally used to calculate spent fuel isotopics, radiation, and heat sources. ORIGEN-S performs the point depletion analysis for the module, relying on other SCALE codes to obtain the burnup-dependent flux spectrum required to generate burnup-dependent cross sections. The SAS2H module can be used to create new ORIGEN-S models by skipping the shipping cask analysis. The following sections describe the SAS2H module and the data required to create an ORIGEN

model. Automatic rapid processing (ARP) is a methodology developed to obtain problem dependent ORIGEN-S cross sections through interpolation.

SAS2. SAS2H is the current version of SAS2, the SCALE module for performing fuel depletion and spent fuel shipping cask analysis. The module consists of the following six major codes:

- BONAMI applies the Bondarenko method of resonance self-shielding for nuclides that have Bondarenko data included in their cross sections.

- NITAWL-II performs the Nordheim resonance self-shielding corrections for nuclides that have resonance parameters included with their cross sections on the cross sections that are produced by BONAMI.

- XSDRNPM performs a 1-D discrete-ordinates transport calculation using the cross sections produced by NITAWL-II to produce cell-weighted cross sections for fuel depletion calculations and angular flux data for shielding analysis.

- COUPLE updates the cross section constants included in an ORIGEN-S nuclear data library with data from the cell-weighted cross section library produced by XSDRNPM and applies the weighting spectrum computed by XSDRNPM to update all nuclides in the ORIGEN-S library that were not specified in the XSDRNPM analysis.

- ORIGEN-S performs both nuclide generation and depletion for the specified reactor fuel history. It also generates neutron and gamma sources for the shielding analysis.

- XSDOSE applies the angular flux at the surface of a shipping cask to compute dose rates outside the shipping cask.

Background material on the BONAMI, NITAWL-II, and XSDRNPM modules is presented in Chapter IV.

The SAS2H module also applies the SCALE free-form reading routines, material information processor and SRCALC subroutines. Four data libraries are required: the SCALE cross section libraries, SCALE standard composition library, an ORIGEN-S binary working library, and an ORIGEN-S master photon binary database (Hermann and Parks, 1997:S2.2.1-2).

Description of Method. SAS2H can be used to perform depletion analysis without performing the shipping cask analysis that is unrelated to this research. This description does not include the three-part shielding analysis sequence that would follow the depletion analysis if the shipping cask calculations were performed. The method starts with data specifying the composition, temperatures, geometry, and time-dependent power history of the reactor fuel. For each time-dependent fuel composition the SAS2H sequence performs its one-dimensional neutron transport analysis of the reactor assembly using a two-part procedure that creates two separate unit-cell lattice models based on the input file specifications. The first model is a unit fuel-pin cell that is used to obtain cell-weighted cross sections. The second model represents a larger unit cell (typically an assembly) within an infinite homogenous medium. The neutron flux spectrum, obtained from the second model, is used to determine nuclide cross sections for the specified burn-up dependent fuel composition. The cross sections derived from a transport analysis at each time step are then used by ORIGEN-S in a point–

depletion computation that generates the burnup-dependent fuel

compositions to be used in the next spectrum calculation. This sequence is

then repeated until the entire history of the reactor is completed (Hermann

Figure III-1: SAS2H Flowchart
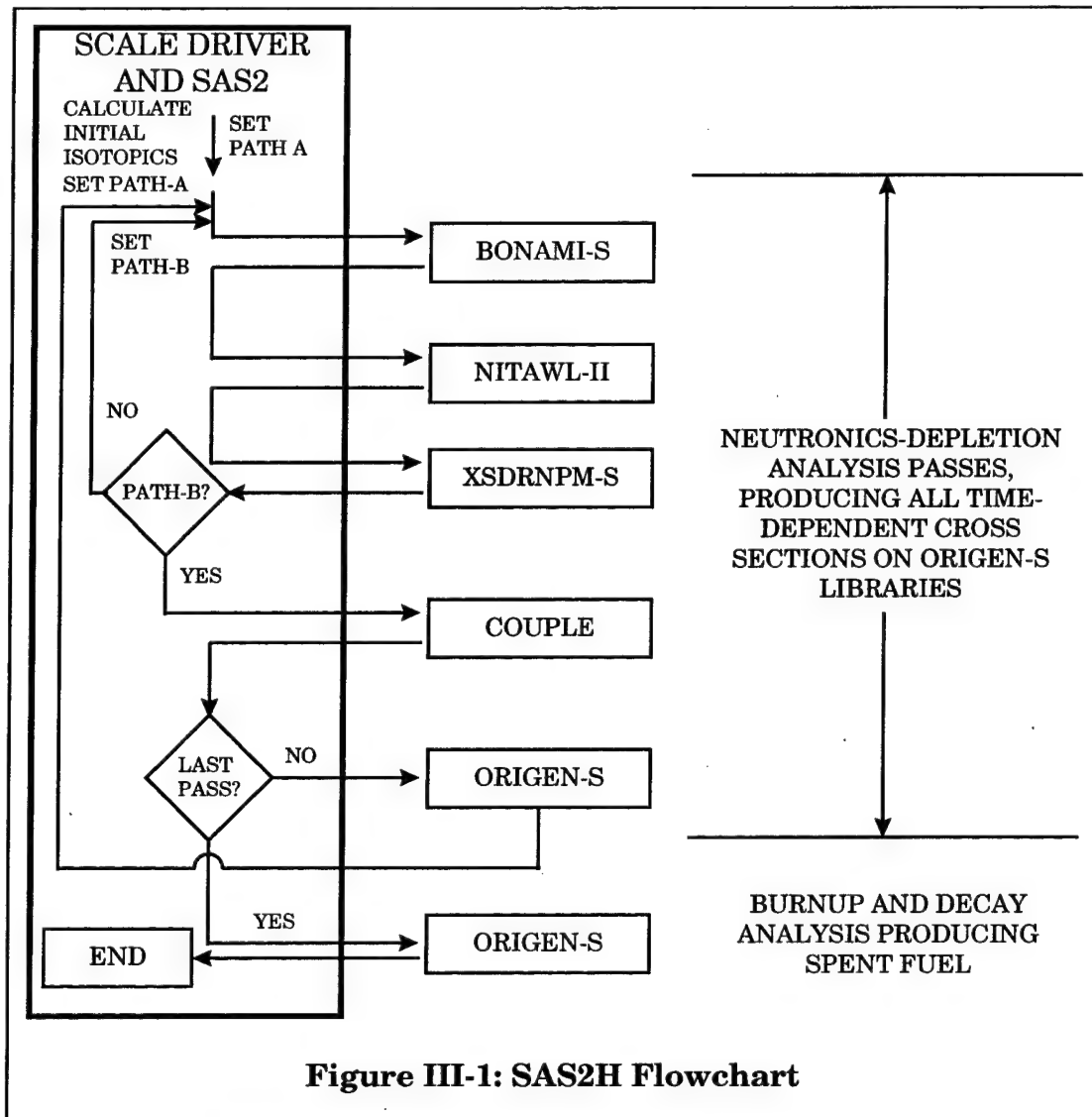
and Parks, 1997:S2.2.1-2).

Preparation of Fuel Cross sections. The original SAS2 model did

not include the larger unit cell model. The updated sequence, SAS2H (Figure

III-1) includes two computational paths (A and B) for the neutronics portion of the depletion analysis. Path A calls BONAMI, NITAWL-II, and XSDRNPM using the fuel-pin cell to produce the cell-weighted cross sections of the fuel zone. Path B calls all five modules using the larger unit cell. After completing the neutronics code computations, COUPLE updates the ORIGEN-S working library with data from the XSDRNPM weighted working library. ORIGEN-S then computes the time-dependent densities of the nuclides in the fuel for the specified power and irradiation times (Hermann and Parks, 1997:S2.2.3).

The path A model represents the fuel as an infinite lattice of fuel pins. Cross sections are processed using a resonance self-shielding analysis followed by a discrete ordinates 1-D transport computation of the neutron flux in a unit cell with white boundary conditions. A white boundary condition is used for cylindrical and spherical geometries when the angular fluxes of all incoming angles on a boundary are set equal to a constant value, such that the net flow across the boundary is zero. Thus, all particles that reach the outer boundary of the cell are reflected back into the cell, and the reflected flux is Lambertian (isotropic over inbound directions). The cell-weighted cross sections produced by the path A model are then applied to the fuel region of the path B model. The larger unit cell used in path B represents either part or all of a reactor fuel assembly. The design of the two unit cells is a principle task of the user. The example presented in the next

chapter describes the process in detail. The SAS2H sequence was developed as an approximate method for evaluating the lateral two-dimensional effects found in non-homogenous fuel-pin lattices. The path B model calculates an *assembly-averaged* fuel region flux that considers the effects due to the path A model and channel moderation (Hermann and Parks, 1997:S2.2.3-5).

Data Processing. The SAS2 control module is used to convert user-input and data from SCALE libraries into the form required by the functional modules. The material information processor prepares isotopic and other material densities using the user input and the contents of the standard composition library. The standard composition library contains over 600 mixtures and isotopes that are commonly used in shielding and criticality problems. The first three input mixtures are used to describe the fuel-pin unit-cell of path A and typically consist of fuel, cladding material, and a portion of the moderator located between the fuel pins. The path A analysis produces the cell-weighted cross sections for the fuel region of the larger unit cell which SAS2H designates as mixture 500 (MX 500). Mixture 500 is applied with other mixtures describing the moderator, control rods, poisons, and structural material to the cylindrical larger unit cell in the path B analysis. After the neutronics calculations are completed using BONAMI, NITAWL-II and XSDRNPM an interface data set is produced for COUPLE that updates cross section constants for libraries used by ORIGEN-S. An

input data set for ORIGEN-S is then created to execute a depletion analysis called a case (Hermann and Parks, 1997:S2.2.5-8).

Fuel Irradiation Analysis. The fuel cross sections vary with burnup because of the change in nuclide concentrations and shift in energy spectrum of the neutron flux. The SAS2H module conducts *passes* through the neutronics-depletion procedure to update the cross sections. The initial passes are used to generate a set of ORIGEN-S libraries, each applicable to a portion of the power history. The final pass is used to perform the depletion analysis. Each pass consists of the following steps:

- Preparation of new data input sets by SAS2

- Return of control to the SCALE driver for execution of the three codes in the path A model

- SAS2 preparation of the code interfaces for the path B model

- Another return to the SCALE driver for execution of the five codes in the path B model

- Return to SAS2

The user-input file specifies the number of irradiation cycles and number of libraries to process for each cycle. The power level, irradiation duration, and reactor downtime are also specified for each cycle in the input file. The fresh-fuel isotopics are used to create the (pass 0) initial library for the first ORIGEN-S case. ORIGEN-S generates the number densities at the midpoint of the first irradiation cycle. The SAS2 module then:

- Computes density-dependent parameters for the resonance calculations

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- Increments the required data set unit numbers (storage locations)

- Adds "pass 1" to the ORIGEN-S library title

- Updates the ORIGEN-S input for the second case to save number densities for the starting point and midpoint of the second irradiation interval

- Rewrites all code interfaces using the new data

Then executing the path A sequence followed by the path B sequence using the new input interfaces produces the pass 1 library. Each additional pass except for the final pass uses the pass 1 procedure of applying the midpoint densities to the neutronics code to produce a new library. The depletion computation applies this library and the densities calculated for the start of the pass. If reactor downtime is specified for the power cycle, a zero power decay computation is performed prior to deriving densities for the next pass. All ORIGEN-S libraries with the exception of the pass 0 library are saved. After all of the ORIGEN-S libraries are generated the final pass uses all libraries and runs through the entire reactor history to perform the depletion analysis. The procedure used for the final pass is to begin by applying the first-cycle power and pass 1 time interval to the pass 1 library. Four equal-sized time steps are used followed by a single downtime interval if specified. The smaller time steps are used because the goal of this pass is accurately calculating nuclide concentrations. A longer time step is adequate for the passes used to generate the cross section libraries. Next a similar calculation is performed using the compositions determined at the end of the pass 1

calculation and the cross section data on the pass 2 library. The procedure continues using each succeeding library and corresponding assembly power and time interval. The schematic of an example of a two cycle case that uses two libraries per cycle is presented as Figure III-2. Ultimately the discharge composition is determined, and is followed by the final decay subcase that is divided into six equal time increments (Hermann and Parks, 1997:S2.2.8,10).

Number densities for the heavy nuclides of the fuel, activation products, and fission products are all computed by ORIGEN-S. The depletion of most light elements including burnable poisons and isotopes of the specified structural materials are also calculated by ORIGEN-S. Densities of alloy and elements in the clad, moderator, or structural materials, and oxygen in the fuel are held constant (Hermann and Parks, 1997:S2.2.9).

Figure III-2: Example of 2 Cycle Case (2 LIB/CYC)

<u>Case Data Requirements.</u> The following data are required to prepare the input files for the SAS2H module:

- fuel, burnable poisons, moderator, cladding, control rods, and structural material: isotopic composition, operating temperatures, density, geometry, and dimensions

- reactor core configuration: geometry and dimensions of fuel elements and control assemblies

- reactor power history: detailed description of all operation cycles including power level, length of irradiation and downtime periods

The following chapter provides background material on the BONAMI, NITAWL-II, and XSDRNPM modules that are used to generate the cross section libraries required by ORIGEN-S. Chapter V then presents an example of the modeling technique using the SAS2H module.

IV. SCALE and ORIGEN-S

Introduction

I chose to use SCALE/ORIGEN-S for the project based on its flexibility, and ability to generate new models rapidly. Although ORIGEN-S does not model the spatial differences of the system as well as ORIGEN2, creating new models is less time and resource intensive. Another advantage is that SCALE is a stand-alone system that does not rely on external codes to create new models. Table IV-1 compares the codes that were considered for the project.

Table IV-1: Code Comparison

Function	Code	Advantages	Disadvantages
Depletion	ORIGEN-S (SCALE)	Speed and ease of model creation	Relies on 1-D calculations
	ORIGEN2	Models derived from multi-dimensional calculations	Model creation is resource intensive
Transport	XSDRNPM (1-D Discrete Ordinates)	Compatibility with ORIGEN-S (SCALE)	Inadequate for systems with axial variations
	VENTURE (Diffusion Theory)	Multidimensional	Output incompatible with ORIGEN2
	MCNP (Monte Carlo based)	Multidimensional	Output incompatible with ORIGEN2

This chapter provides details about the BONAMI, NITAWL-II, and XSDRNPM modules that are used in conjunction with ORIGEN-S in the

SCALE system. These modules create the ORIGEN-S problem dependent cross section library from generic multi-group cross section data. First, BONAMI applies a Bondarenko resonance self-shielding correction to the generic cross sections. NITAWL-II then applies an additional resonance self-shielding correction based on the Nordheim Integral Treatment. XSDRNPM then uses the corrected cross sections to perform a 1-D transport calculation to produce cell-weighted cross sections.

Bondarenko Resonance Self-Shielding (Greene, 1997:F1.2.1-2)

In performing multigroup resonance self-shielding calculations it is desirable to calculate effective cross sections in the form

$$\overline{\sigma_g} = \frac{\int_g du\, \sigma(u)\phi(u)}{\int_g du\, \phi(u)}, \tag{16}$$

where lethargy, u, is defined by changes in energy produced by elastic scattering. Lethargy relates the energy, E, and reference or maximum energy, E_0, of a neutron using the relation

$$u(E) = \ln\frac{E_0}{E} \tag{17}$$

As the cross section, $\sigma(u)$, is generally known, resonance self-shielding involves a determination of the flux, $\phi(u)$. The Bondarenko method is based on the simple expression for the flux in an infinite homogenous medium,

$$\phi(u) \sim \frac{1}{\Sigma_t(u)}, \tag{18}$$

where $\phi(u)$ is the flux per unit lethargy u, and $\Sigma_t(u)$ is the macroscopic total cross section. The expression for the collision density in an infinite medium having a small absorption cross section can be reduced through a series of assumptions to the form of Equation (18) (Greene, 1997:F1.2.1). A more direct method is to invoke the narrow resonance approximation which assumes that collision density, $F(u)$, is unaffected by a very narrow resonance and is therefore, constant:

$$F(u) \equiv \Sigma_t(u)\phi(u) = \text{constant} \tag{19}$$

For the Bondarenko approach, Equation (18) is substituted in Equation (16) to form the expression

$$\overline{\sigma^i_g} = \frac{\int_g du \dfrac{\sigma^i(u)}{\Sigma_t(u)}}{\int_g du \dfrac{1}{\Sigma_t(u)}}, \tag{20}$$

or equivalently,

$$\overline{\sigma^i_g} = \frac{\int_g du \dfrac{\sigma^i(u)}{N_i \sigma^i_t(u) + \sum\limits_{j \neq I} N_j \sigma^j_t(u)}}{\int_g du \dfrac{1}{N_i \sigma^i_t(u) + \sum\limits_{j \neq I} N_j \sigma^j_t(u)}}, \tag{21}$$

where i designates the nuclide of interest, N is the nuclide number density, and σ_t is the microscopic total cross section. Dividing the numerator and denominator of Equation (21) by N_i, and defining $\sigma^i_0(u)$ as

$$\sigma^i_0(u) \equiv \sum_{j \neq i} N_j \sigma^j_t(u)/N_i, \tag{22}$$

yields the equivalent formula:

$$\overline{\sigma_g^i} = \frac{\int_g du \dfrac{\sigma^i(u)}{\sigma_t^i(u) + \sigma_0^i(u)}}{\int_g du \dfrac{1}{\sigma_t^i(u) + \sigma_0^i(u)}}. \tag{23}$$

The $\sigma_0^i(u,T)$ term is the cross section per atom of the nuclide i for all nuclides in the mixture other than nuclide i itself. The cross sections for the specific process implied by Equation (23) are a function of three variables other than the nuclide's cross section:

        (1) energy group,

        (2) temperature (Doppler broadening), and

        (3) σ_0^i.

The Bondarenko method discounts some fine structure by using an effective constant value for σ_0 within an energy group. This method allows the calculation of cross sections without the details of the compositions in which they may be used. The infinite dilution average for a process is defined by evaluating Equation (23) for $\sigma_0 = \infty$:

$$\overline{\sigma_g^{ID}} = \frac{\int_g du \, \sigma(u)}{\int_g du}. \tag{24}$$

For a finite value of σ_0 and temperature T, the Bondarenko factors, $F_g^i(\sigma_0,T)$, are defined as follows

$$\overline{\sigma_g^i}(\sigma_0,T) \equiv F_g^i(\sigma_0,T)\overline{\sigma_g^{ID}}. \tag{25}$$

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BONAMI is a module that computes values of cross sections by interpolating between values of tabulated data at several values of σ_0 and temperature.

Nordheim Resonance Self-Shielding (Greene, Petrie, and Westfall, 1997: F2.1.1-F2.2.2)

The Nordheim Integral Treatment provides an approximation for the energy dependence of the neutron flux in a material region containing a resonance absorber and up to two additional admixed moderators. The material region may be infinite or may correspond to a 1-D slab, cylinder, or sphere surrounded by a moderator medium where the neutron flux is spatially flat and varies slowly with energy. Dancoff factors are used to account for the presence of more than one absorber lump in the moderating medium. They approximate the effect that one absorber has on the self-shielding of another absorber in close proximity. The presence of additional absorber lumps is to vary the flux seen by the individual absorber lump and create additional self-shielding. A Dancoff factor of zero represents a single absorber lump isolated in a moderator medium, while a Dancoff factor of 1.0 represents an infinite medium of absorber with no external moderator present. Nordheim's method approximates the collision density as a function of neutron energy, E, as

$$\phi(E)\Sigma_T(E) = \sum_{i=1}^{3}\left[(1-P_0^*(E))\int_E^{E/(1-\alpha_i)}\phi(E')\Sigma_{si}(E')\frac{dE'}{\alpha_i E'} + P_0^*(E)\Sigma_{Ti}(E)W(E)\right], \quad (26)$$

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where:

$\phi(E)$ is the neutron flux (n-cm/cm³-s);

$\Sigma_T(E)$ is the macroscopic total cross section in the absorber (cm⁻¹);

i is the nuclide index(1 for the absorber, 2 for the first admixed moderator, 3 for the second admixed moderator);

$P_0^*(E)$ is the Dancoff-corrected, first-flight escape probability for the absorber region, $P_0^*(E) = P_0(E)(1-C)/\left\{1 - [1 - \Sigma_T(E)\bar{r}P_0(E)]C\right\}$, $P_0(E)$ is the escape probability of Case, deHoffman, and Placzek, C is the Dancoff factor, $\Sigma_T(E)$ is the total cross section of the absorber medium, and $\bar{r}$ is the mean chord length (4 volume/surface) of the absorber region;

α_i is the maximum fractional energy loss a neutron can suffer in an elastic collision with a nuclide of mass A_i, $\alpha_i = 4A_i/(A_i+1)^2$;

Σ_{Ti} and Σ_{si} are the macroscopic total and elastic-scattering cross sections of nuclide i, (cm⁻¹); and

$W(E)$ is the assumed energy variation of the neutron flux in the external moderator region. (In the thermal energy range, $E < 5\,kT$, $W(E)$ is approximated by the Maxwellian distribution, CE/(kT)² exp[-E/kT], where C is the normalization constant, exp[5]/25, k is the Boltzmann constant 8.61664×10⁻⁵ eV/K, and T is the temperature of the medium in Kelvin, above the thermal range, $W(E)$ is approximated as $\frac{1}{E}$.)

The first term on the right-hand side of Equation (26) is the collision density in the absorber region due to sources arising from isotropic elastic scattering at energies E' above E. The second term is the collision density due to the flux at the absorber-moderator boundary penetrating into the absorber region. The model incorporates several approximations:

- Each resonance nuclide can be treated independently of other resonance nuclides that may be present in the system. This prevents taking *resonance overlap* between nuclides into account.

- The neutron flux is spatially uniform in the absorber and moderator regions.

- Neutron transport into and out of the absorber region can be treated with first-flight escape probabilities.

- The Dancoff factor accounts for the presence of other absorber lumps in the system. This factor corresponds to the first-flight transmission probability across the moderator.

NITAWL-II is the SCALE module that applies the Nordheim Integral Treatment to perform problem-dependent resonance self-shielding.

<u>One-Dimensional Discrete-Ordinates Transport</u> (Greene and Petrie, 1997:F3.2.1)

The time-independent Boltzmann transport equation can be written

$$\bar{\Omega} \cdot \nabla \psi(\bar{r}, E, \bar{\Omega}) + \Sigma_t(\bar{r}, E) \psi(\bar{r}, E, \bar{\Omega}) = S(\bar{r}, E, \bar{\Omega}). \qquad (27)$$

Equation (27) balances the streaming losses (first term) and collision losses (second term) with a source (right hand side) of neutrons at each point in space, $\bar{r}$, energy, E, and direction of motion, $\bar{\Omega}$, per unit volume, energy, and solid angle, to determine the flux, given the cross sections, boundary conditions and fixed sources (emitters). The source term consists of three components:

the scattering source, $S(\bar{r}, E, \bar{\Omega})$,

the fission source, $F(\bar{r}, E, \bar{\Omega})$, and

a fixed source, $Q(\bar{r}, E, \bar{\Omega})$.

The scattering source is expressed as

$$S(\bar{r},E,\bar{\Omega}) = \int_0^{4\pi} d\bar{\Omega}' \int_0^\infty dE' \Sigma_s(\bar{r},E' \to E, \bar{\Omega}' \to \bar{\Omega}) \psi(\bar{r},E,\bar{\Omega}'))$$ (28)

while the fission source term is typically written

$$F(\bar{r},E,\bar{\Omega}) = \frac{1}{4\pi k} \chi(\bar{r},E) \int_0^{4\pi} d\bar{\Omega}' \int_0^\infty dE' \nu(\bar{r},E') \Sigma_f(\bar{r},E') \psi(\bar{r},E',\bar{\Omega}')$$ (29)

where:

$\Sigma_s(\bar{r},E \to E, \bar{\Omega}' \to \bar{\Omega})$ is the macroscopic scattering cross section per unit energy for scattering from energy E' to E and from direction $\hat{r}'$ to $\hat{r}$;

$\chi(\bar{r},E)$ is the fraction of fission neutrons per unit energy produced at $\bar{r}$ and E;

$\nu(\bar{r},E)$ is the average number of neutrons produced per fission;

$\Sigma_f(\bar{r},E)$ is the macroscopic fission cross section;

k is the effective multiplication constant; and

neutrons emitted from fission are emitted isotropically.

With this form of fission source term, the transport equation is an eigenvalue equation with ψ as the eigenfunction and k as the eigenvalue.

Three coordinate systems (slab, cylindrical, and spherical) are typically used for one-dimensional calculations. It is traditional to calculate as a function of angles expressed in cosine units, $\mu = \cos\phi$. The discrete-ordinates method approximates the integrals found in the source terms as weighted sums.

XSDRNPM is a module that performs 1-D discrete-ordinates calculations in slab, cylindrical, or spherical geometries. It is used to determine fluxes through spectrum calculations using the pin-cell and larger unit cell models and to collapse cross sections to produce the ORIGEN-S problem dependent libraries.

V. Modeling the OSU Research Reactor

Overview

An ORIGEN-S depletion analysis of the OSURR was conducted to demonstrate the modeling methodology. The process involved the collection of design and operating data and the creation of an input file for the SAS2H module of SCALE4.3.

The Ohio State University Research Reactor

The research reactor was selected as an example due to its proximity and accessibility. The reactor is a pool-type light water reactor that is licensed for 500KW maximum power. The reactor was originally fueled with highly enriched uranium, but was refueled in 1988 following consultation with the National Organization of Test, Research, and Training Reactor Operators. The new fuel was developed as part of the Reduced Enrichment for Research and Test Reactors (RERTR) fuel development program of the Argonne National Laboratory. The new fuel that was selected is uranium enriched to 19.5% $^{235}_{92}U$, in the form of uranium-silicide (U_3Si_2) particles dispersed in an aluminum matrix. The generic cross section libraries that are supplied with ORIGEN2 and ORIGEN-S are not applicable to the research reactor due to the unusual fuel and core geometry. This example provides an opportunity to demonstrate the flexibility of the SCALE system

in creating a problem dependent cross section library and performing a depletion analysis of the RERTR fuel assemblies.

Core Description

The reactor core consists of a 5 by 6 array of fuel assemblies. The reactor fuel is manufactured into fuel plates. Several fuel plates are mounted together to form a fuel assembly. The fuel assemblies are in turn mounted into a core grid plate forming the core structure. The central irradiation facility (CIF) occupies the center position of the grid while four control rod fuel assemblies occupy the grid locations at the corners of the CIF. The remaining 25 grid locations are filled with fuel assemblies. There are four types of fuel assemblies:

- Standard-full uranium loading (assembly designator is **OH**).

- Control-middle plates removed to create a gap for control rods (assembly designator is **OHC**).

- Partial-physically identical to standard assemblies except that some fuel plates do not contain uranium. Available in 25, 37.5, 50, and 62.5 percent of nominal uranium loading of standard fuel assembly (assembly designator is **OHP**).

- Dummy-none of the fuel plates contain uranium (assembly designator is **OHF**).

Replacing standard fuel assemblies with partial or dummy assemblies can vary the core uranium loading to meet experiment needs. I chose to model the most common core configuration, designated LEU Core #3 by the reactor operating staff, shown in Figure V-1. The Babcock & Wilcox Company

supplied the reactor fuel assemblies under the terms of the DOE Fuel

Assistance Program managed by EG&G Idaho, Inc.

	A	B	C	D	E
1	OHF-001	OH-002 199.83	OH-003 199.84	OH-004 199.76	OHF-002
2	OH-006 199.83	OHC-001 124.89	OH-007 199.82	OHC-002 124.86	OH-008 199.83
3	OH-009 199.84	OH-010 199.84	CIF	OH-011 199.87	OH-012 199.85
4	OH-013 199.85	OHC-004 124.89	OH-014 199.84	OHC-003 124.89	OH-015 199.83
5	OHF-004	OHP-004 124.89	OH-018 199.71	OH-019 199.84	OH-020 199.84
6	OHF-005	OHF-006	OHF-007	OHF-008	OHF-009

NUMBER UNDER ASSEMBLY DESIGNATOR = U-235 LOADING (g)

TOTAL CORE U-235 LOADING = 3821.65 g

Figure V-1: LEU Core #3

The active portion of fuel, or *meat*, is contained in the center of a flat, 0.050" thick, aluminum-6061 alloy plate. The plates are attached to aluminum side plates to form a 3" by 3" fuel assembly. The lower end box is found at the bottom of each assembly, and is used to mount the assemblies on the grid plate.

A standard fuel assembly, shown in Figure V-2, consists of 18 plates, 16 containing uranium fuel and 2 outer dummy plates. The partial assemblies have some fuel plates replaced with pure aluminum alloy. The dummy assemblies have no plates loaded with uranium fuel.
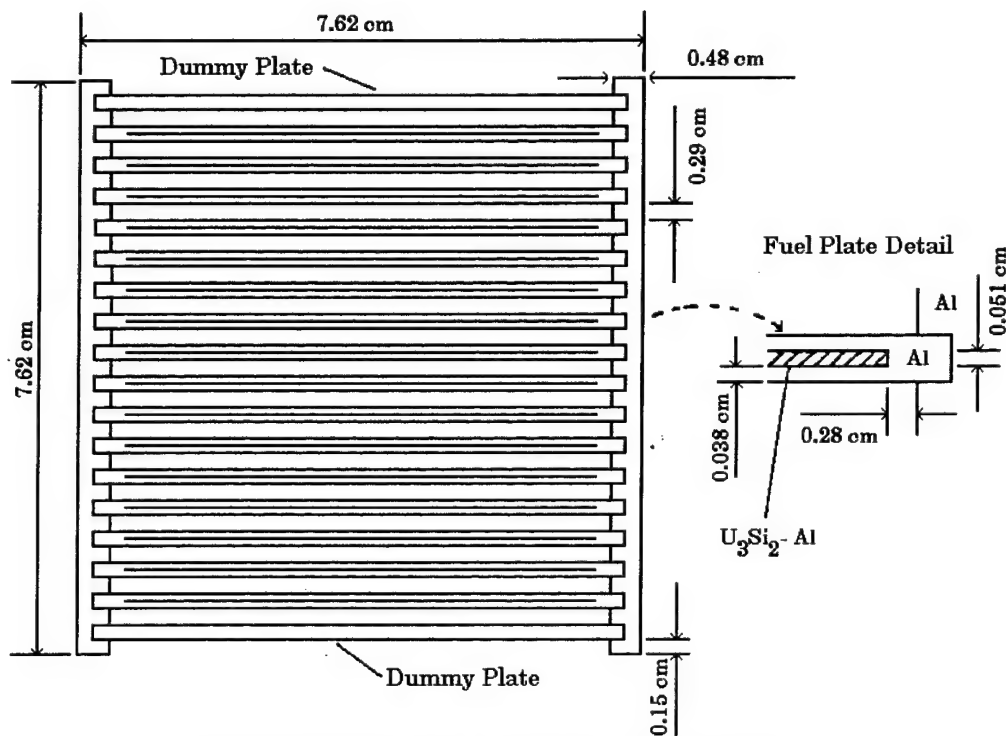
Figure V-2: Standard Fuel Assembly

The control rod fuel assemblies, shown in Figure V-3, are constructed of the same fuel plates as the standard assemblies. A gap for the control rods

is created in the center of the assembly by removing 6 of the inner plates. The OSURR uses three shim-safety rods and one regulating rod (Figure V-4) to control reactivity. All of the rods are oval in cross section, but differ in composition. The safety rods are solid and manufactured from type 304 stainless steel with 1.5 percent natural boron. The safety rods are fluted to improve heat dissipation The regulating rod is a hollow type 304 stainless steel rod. To avoid water-hole power peaking in the plates adjacent to the rod channel (while the rod is withdrawn), these two fuel plates are dummy plates.
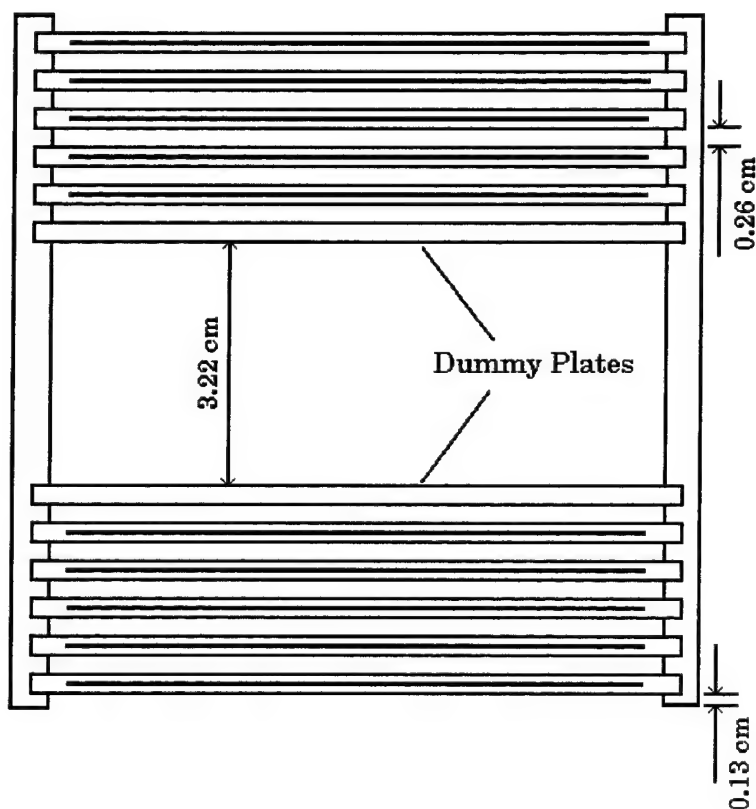
Figure V-3: Control Rod Fuel Assembly

Shim-Safety Rod

Regulating Rod
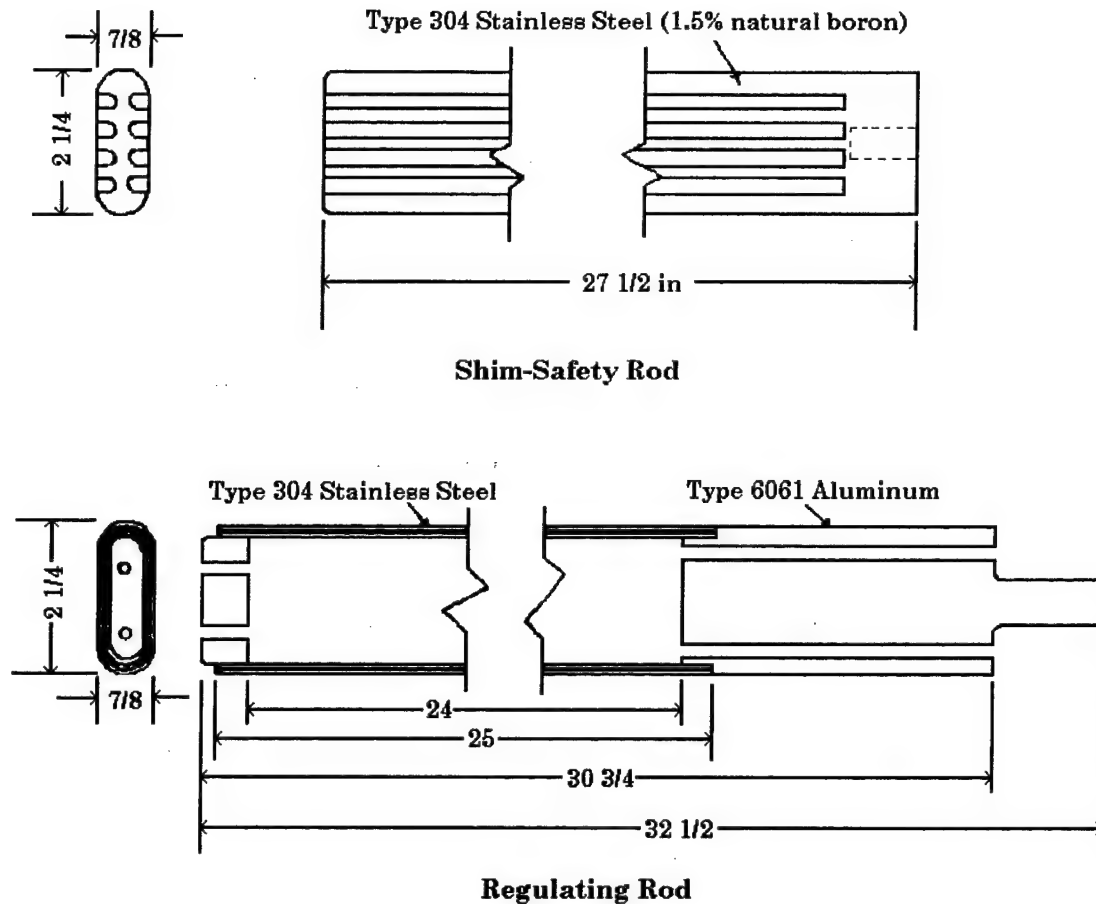
Figure V-4: Control Rods

SCALE Input File Preparation

The SCALE input file specifies which subroutines are to be executed,

which cross section libraries are to be used, material compositions, operating

temperatures, core geometry, and power history. The majority of the data

required to create the input file was obtained from the Safety Analysis Report

and Technical Specifications for the OSURR and from blueprints. A one-

dimensional heat transfer analysis was performed to determine the average

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temperatures of the fuel meat and cladding. Four steps were performed to convert the data into an input file after collecting the reactor design and operating data:

- determine the initial isotopics;
- design the pin cell;
- design the larger unit cell; and
- specify the reactor power history in cycle format.

The first step was a straightforward calculation of the initial isotope concentrations based on the fuel and material specifications. After the isotopic compositions of the reactor core components were calculated, the next step was to specify the geometry of the pin cell model that SAS2H uses to determine the cross sections of the fuel zone during the path A calculations. The third step was to specify the cylindrical larger unit cell that was used to determine burnup dependent cross sections during the path B calculations. The final step was the creation of a power history that represented the nine years of operation of the OSURR following the refueling that occurred in 1988. The input file is organized into data blocks, which will be discussed in the sequence that they appear in the input file. Appendix A: SAS2 Input Data Requirements contains a detailed description of the input files.

Data Block 1. Format

=SAS2   PARM=

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Example:

=SAS2   PARM=(HALT09,SKIPSHIPDATA)

This block specifies SAS2H as the module activator and specifies the
parameters HALT ii and SKIPSHIPDATA. These parameters instruct the
SAS2H module to omit the shipping cask analysis portion of the routine. The
characters *ii* that follow the HALT parameter instruct the SCALE driver to
terminate the case after the ii-th pass. For the example case, ii was
computed by multiplying the number of cycles (NCYCLES) by the number of
cycles per library (NLIB/CYC) which determines the total number of passes
used in the specified power history.

<u>Data Block 2.</u> Format:

TITLE

Example:

OHIO STATE RESEARCH REACTOR: MODEL ONE

This block contains the 80-character title for the case.

<u>Data Block 3.</u> Format:

LIB GE

Example:

44GROUPNDF5   LATTICECELL

This block specifies the SCALE library (LIB) and reactor lattice
type (GE). The reactor lattice must be designated as LATTICECELL for
all SAS2H calculations. The SCALE documentation recommends the 44-

group library derived from the ENDF/B-V data (44GROUPNDF5) which was chosen for the example case. This library is designed for LWR analysis and has been extensively validated against LWR critical experiments (Jordan and Bowman, 1997:M4.1.1). Nine different cross section libraries are provided with SCALE. The libraries differ in the neutron energy group structure, ranging from 16 to 238 groups. Six of the libraries were designed primarily for criticality analysis, the other three were developed as shielding libraries.

Data Block 4. Format:

SC MX END END COMP

Example:

```
ARBMU3SI2AL 3.0 3 1 0 0 92000 22.01 14000 1.76 13027
76.23 1 1 329.56 92234 0.149 92235 19.5 92238 80.351 END
ARBMAL6161 2.7 8 1 0 0 13027 97.4 12000 1.0 14000 0.6
29000 0.3 24000 0.2 26000 0.35 25055 0.075 22000 0.075 2 1
329.53 END
H2O 3 325.3 END
SS304 4 325.3 END
ARBMSAFEROD 7.84 5 1 0 0 24304 19.0 25055 2.0 26304
67.5 28304 9.5
5000 1.5 5 1 325.3 END
END COMP
```

This block specifies the material composition characteristics. Five different mixtures were created for the example problem: U_3Si_2-Al matrix (fuel meat), aluminum 6161 alloy, water, type 304 stainless steel, and the stainless steel-boron mixture of the safety rods. The density, isotopic

composition, and average temperature are specified for each mixture using the SCALE material information processor format:

SC ROTH NEL IVIS ICP IRS NCZA ATPM (entry 1)
MX DEN= VF ADEN TEMP IZA WTP END (entries 2-7)

If a material is included in the SCALE standard composition library its standard composition component name (SC) is the only requirement for entry 1. The remaining variables of entry 1 are used to define arbitrary materials, which are materials that are not included in the standard composition library.

An arbitrary material is defined when the SC begins with *ARBM*. The theoretical density (ROTH) (g/cc) and number of elements (NEL) are declared next. The IVIS and IRS variables are no longer used but 1 or 0 must still be entered for each. The ICP variable is used to declare the mixture a chemical compound (1) or an alloy (0). The NCZA and ATPM variables are entered as a pair for each element declared by NEL. The element is first identified by its identification number (NCZA). The material information processor and standard composition library use ID numbers to identify elements, nuclides, and isotopes. A nuclide is identified by an ID number computed by the formula A+1000*Z, where Z and A are the charge and mass numbers for the nuclide. Elements with isotopic mixtures (typically natural abundance) have ID numbers of Z*1000 (Petrie, Fox, and Lucius,1997:M8.2.1) The ATPM variable is then used to declare the number of atoms of this element per

molecule if the arbitrary material is a chemical compound (ICP=1), or the weight percent of this element if the arbitrary material is an alloy (ICP=0).

The mixture identification number (MX) is always required, as is the END keyword which terminates a standard composition. The remaining entries are optional. The density multiplier (VF) (density fraction, volume fraction, or a combination) has a default value of 1; a different value can be specified if needed. The number density (ADEN) (atom/b-cm) for the nuclide is only required if VF=0. The temperature (TEMP) of the mixture has a default value of 293K. The sixth entry is used for nuclides that have multiple isotopes. The entry consists of isotope ID numbers (IZA) and weight percents (WTP) entered as pairs. An IZA/WTP pair is required for each isotope in a multiple isotope nuclide.

Data Block 4 is terminated by the keywords END COMP following the last mixture description.

Mixture 1 (U_3Si_2-Al). This mixture was designated ARBMU3SI2AL. The IAEA research reactor core conversion guidebook states that the density of U_3Si_2 is 12.2 g/cm^3 and the porosity content of fuel cores produced by Babcock & Wilcox ranged from nine to ten percent by volume (Matos and Snelgrove, 1992:I-6.1). The density (ROTH) of the fuel meat was calculated to be 3.0 g/cm^3 using 9.5 vol-% porosity. The composition specifies that the mixture is composed of three elements (NEL=3). The SCALE material information processor no longer uses the

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IVIS and IRS variables, but 1 and 0 must still be entered for each respectively. The ICP variable is given the value 0 to indicate that the fuel mixture is an alloy and not a chemical compound. The initial fuel meat isotopic content by weight is 22.01% uranium (^{238}U-80.3%, ^{235}U-19.5%, ^{234}U-.2%), 1.76% silicon, and 76.23% aluminum. The VF variable is specified as 1 indicating that the fuel is not compressed. A heat transfer analysis, described in Appendix B, predicted that the average fuel meat temperature was 329.56K under 500KW operation.

Mixture 2 (AL6161). This mixture was designated ARBMAL6161. A density of 2.7 g/cm^3 and composition of 97.9% Al, 1.0% Mg, 0.6% Si, 0.3% Cu, and 0.2% Cr were specified in accordance with the *10th Edition Metals Handbook* (ASM International, 1990:102-103). The *Metals Handbook* also specifies a maximum of 0.25% Zn, however the zinc isotopes are not included in the SCALE cross section library and their inclusion results in a fatal error. Therefore, zinc was omitted from the analysis. The heat transfer analysis in Appendix B predicted that the average clad temperature was 329.53K.

Mixture 3 (H$_2$O). Water is a standard mixture provided in the standard composition library provided with SCALE and is designated H2O. The OSURR Safety Analysis Report contains a heat transfer analysis that predicts the average moderator temperature to be 325.3K during 500KW operation (Ohio State University, 1987:109).

Mixture 4 (Type 304 Stainless Steel). This alloy is also provided in the standard composition library and is designated SS304. The SS304 standard composition has a density of 7.92 g/cm^3 and consists of 19.0% Cr, 2.0% Mn, 69.5% Fe, and 9.5% Ni. The moderator temperature, 325.3K, was specified as the temperature of the regulating rod.

Mixture 5 (Safety Rod). This mixture was designated ARBMSAFEROD. The mixture was created by adding 1.5-% boron to SS304, resulting in an alloy with a density of 7.84 g/cm^3. Again the moderator temperature of 325.3K was used to specify the temperature of the safety rods.

Data Block 5. Format:

CPT PITCH FUELOD MFUEL MMOD CLADOD MCLAD CLADID MGAP END

Example:

SYMMSLABCELL 0.417 0.051 1 3 0.127 2 END

This block specifies the geometry of the fuel pin-cell (Figure V-5) used for the path A calculations that determine the cross sections of the fuel zone of the larger unit cell. The dimensions that were used were taken from the OSURR Safety Analysis Report and Technical Specifications. The CPT variable specifies the type of lattice that will be used for the pin cell model. The available lattice options are:

- SQUAREPITCH-used for an infinite array of cylinders arranged in a square lattice

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- TRIANGPITCH-used for an infinite array of cylinders arranged in a triangular lattice

- SYMMSLABCELL-used for an infinite array of symmetric slab cells
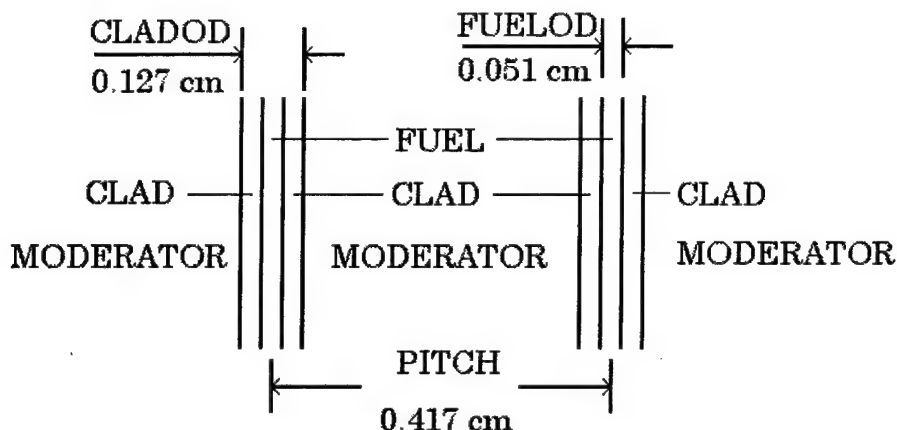
Figure V-5: Fuel-Pin Cell

The CPT variable was designated as SYMMSLABCELL to specify the pin cell as symmetric slab. The pitch between plates (PITCH) indicates center-to-center spacing (cm) between fuel pins or slabs. The width of the fuel region is specified by the FUELOD variable. The CLADOD variable specifies the outer dimension of the clad material. The mixture numbers for the fuel cell compositions are fuel (MFUEL= 1), clad (MCLAD= 2), and moderator (MMOD= 3). The variables CLADID and MGAP that specify the clad inner dimension and gap mixture number respectively were omitted for the example because there is no gap between the fuel and clad regions of the fuel plates.

Data Block 6. This block is used to change default values for parameters used to control the XSDRNPM module. The default values were used for the example.

Data Block 7. Format:

NPIN/ASSM= FUELNGTH= NCYLES= NLIB/CYC= LIGHTEL= PRINTLEVEL= VOLFUELTOT= INPLEVEL= NUMHOLES= NUMINSTR= MXTUBE= ORTUBE= SRTUBE= ASMPITCH= NUMZTOTAL= MXREPEATS= MIXMOD= BPRNUM= GTHOLENUM= FACMESH= LIMINTGEO= END

Example:

NPIN/ASSM=16 FUELNGTH=60.96 NCYCLES=10 NLIB/CYC=1 PRINTLEVEL=5 LIGHTEL=5 VOLFUELTOT=303.36 INPLEVEL=2 NUMZTOTAL=7 END

This block specifies the larger unit cell composition and desired level of output detail. The number of fuel plates per assembly (NPIN/ASSM) was specified as 16 to represent a standard fuel assembly and as 10 to represent a control fuel assembly. The active fuel length (FUELNGTH) of all assemblies is 60.96 cm. The number of irradiation cycles (NCYCLES) varied from 9 to the maximum of 25. The overall core power history was represented by seven distinct variations in order to investigate its impact on the output. With the exception of the power history that represented constant low power continuous operation and used nine libraries, all other cases used one cross section library per cycle (NLIB/CYC=1). The output detail level was set to PRINTLEVEL=5, the minimum necessary to specify light elements,

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actinides, and fission product compositions in grams. The light elements (LIGHTEL) that are found in the aluminum alloy end plates and cladding of the fuel plates are included in the analysis by designating the number of elements in Data Block 7. Data Block 10 is used to identify them and provide masses for them. The total fuel volume per assembly (VOLFUELTOT) was specified as 303.36 cm^3 for a standard fuel assembly, and 189.60 cm^3 for the control fuel assemblies. The inclusion of INPLEVEL=2 allows the larger unit cell to be user-specified rather than using the default configuration.

Several limitations of SAS2H created problems during the design of the larger unit cell. The module uses a cylindrical larger unit cell within an infinite homogenous medium during the path B calculations. The first limitation is that the code is limited to a single type of cell. This creates the dilemma of representing the CIF, standard, partial, and the control fuel assembly with a single unit cell. Additionally there was concern that the small OSURR was not as homogenous as the large commercial reactors for which the code was designed. Another limitation is that unlike the fuel-pin cell model (path A), the user can not choose the lattice type of the larger unit cell (path B). This constraint forces the four types of square fuel assemblies to be represented by a single cylindrical larger unit cell. Brian Broadhead of the Computational Physics and Engineering Division of ORNL recommended the creation of a core averaged cell to overcome these limitations (Broadhead,

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1997). Five different cells were designed to represent the core in order to evaluate the impact of varying the design of the larger unit cell.
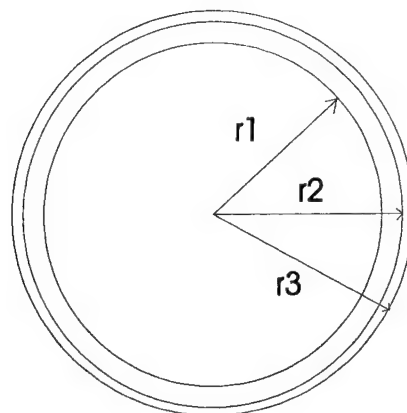
ZONE	MX	RADIUS (cm)
Fuel	500	r1=3.708
Assembly	2	r2=4.076
Channel Moderator	3	r3=4.213

Figure V-6: Standard Fuel Assembly Cell

Standard Fuel Assembly Cell. This cell (Figure V-6), designed to represent the standard fuel assembly, is composed of three zones. A cell-weighted fuel zone (MX 500) which results from the pin cell calculations forms the center of the cell. A zone of assembly casing (MX 2) surrounds the fuel. This zone represents the aluminum alloy found in the side and dummy plates of the assembly. The outermost zone represents the channel moderator (MX 3) between assemblies. The zone radii were calculated from region cross-sectional areas to convert the square fuel assembly to the cylindrical larger unit cell that is required by SAS2H.
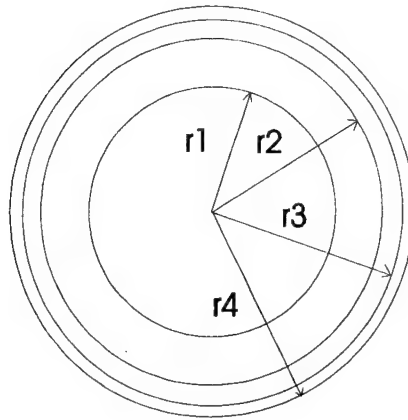
ZONE	MX	RADIUS (cm)
Moderator	3	r1=2.613
Fuel	500	r2=3.708
Assembly	2	r3=4.076
Channel Moderator	3	r4=4.213

Figure V-7: Control Fuel Assembly Cell

Control Fuel Assembly Cell. This cell (Figure V-7) consists of four zones and represents the control fuel assembly. The safety and regulating rods were purposely omitted from the cell because an infinite medium of cells containing rods would not represent the OSURR core. The cell consists of a zone representing the moderator (MX 3) filling the space of the removed inner fuel plates. The innermost zone is surrounded by the cell-weighted fuel zone (MX 500), assembly casing zone (MX 2), and channel moderator (MX 3).

Core Average Cells. Three core average cells (Figure V-8) were designed to represent reactor operation at 5, 250, and 500KW. The core

average models were designed at different power levels to reflect the changes in control rod withdrawal from the active fuel region with power level. The control rod fuel assemblies posed a challenge when designing the core average larger unit cell because the SAS2H model assumes that the core is composed of an infinite lattice of larger unit cells and only four assemblies contained control rods. The approach used in designing the core average cells was to sum the total volume of the control rods in the active fuel region of the core and then divide it equally among the fuel assemblies. The five dummy fuel assemblies that form row 6 of the core were not considered when determining the core average cell, leaving a total of 25 assemblies. The volumes of control rods in the active fuel region were calculated using the rod withdrawal lengths for 5 and 500 KW operation, and interpolated values for 250 KW. The innermost zone of the core average larger unit cell represents the moderator (MX 3) that fills the hollow regulating rod. The area was computed by taking the area of the hollow zone of the rod and dividing it by 25 (total number of core assemblies). The second zone represents the regulating rod (MX 4), with its area computed in a similar fashion as the first zone. The third zone represents the three safety rods (MX 5). The areas of the control and regulating rods were calculated for reactor operation at 5, 250, and 500KW. The fourth zone represents the moderator (MX 3) between the control rods and the innermost set of fuel plates in a control fuel assembly. The fifth zone is the cell-weighted fuel zone (MX 500) which

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represents a core average of 20 standard fuel assemblies and 4 control fuel assemblies. The last two zones represent the assembly casing (MX 2) and channel moderator (MX 3) between core assemblies.
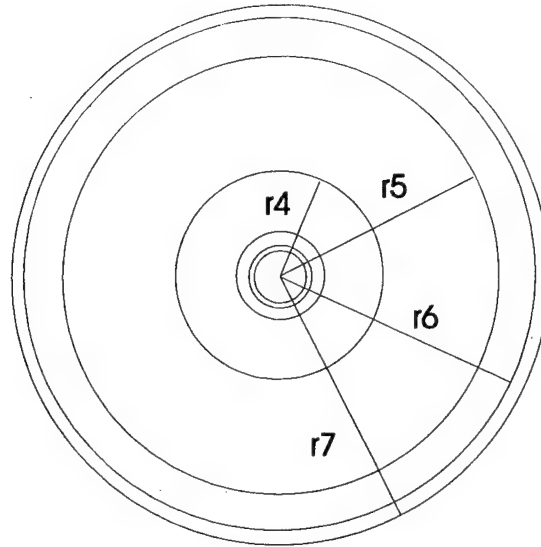
Zone	MX	RADIUS(cm)	5KW	Power 250KW	500KW
Moderator	3	r1=0.2762			
Reg. Rod	4		r2=0.3100	r2=0.3133	r2=0.3167
Safety Rods	5		r3=0.4713	r3=0.4655	r3=0.4604
Moderator	3	r4=1.1185			
Fuel	500	r5=3.5304			
Assembly	2	r6=3.9152			
Moderator	3	r7=4.0570			

Figure V-8: Core Average Cells

Several other variables (NUMHOLES, NUMINSTR, MXTUBE, ORTUBE, SRTUBE, ASMPITCH, MIXMOD, BPRNUM, FACMESH, LIMINTGEO) can be used in data block 7 to include burnable poisons,

instrument holes, or a second type of fuel pin in the larger unit model. None of these variables were applicable to the research reactor.

Data Block 8. Format:

MIX RADIUS

Example:

3 .2762 4 .3133 5 .4655 3 1.1185 500 3.5304 2 3.9152 3 4.0570

This block specifies the MIX and RADIUS (cm) of each zone of the larger unit cell. The MIX/RADIUS pairs begin with the inner zone and work outward. If each power cycle does not use the same fuel configuration (MXREPEATS=0), the pairs must be entered NCYCLES*NLIB/CYC times.

Data Block 9. Format:

POWER= BURN= DOWN= END

Example:

POWER=0.000279 BURN=3283.75 DOWN=0 END
POWER=0.013 BURN=.25 DOWN=1. END

This block specifies the power history for the case. The POWER (MW/Assembly), irradiation duration (BURN) in days, and decay duration (DOWN) in days are input for each cycle that is identified in Data Block 7. The constraint of having only 25 total cycles to represent nine years of daily operation posed another problem. The reactor is operated based on research requirements. It is only operated during weekdays and rarely at night. The 25-cycle limitation prevented an exact representation of the OSURR operating history. Seven different power histories were created to simulate

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the same total power production, varying from continuous low power operation to a series of maximum power/shutdown intervals. Details of these power histories are presented in chapter VII.

Data Block 10. Format:

EL WTLITE

Example:

AL 2.8293 MG .0289 SI .01734 CU .00867 CR .00578

This block specifies the masses (kg per assembly) of each light element that was designated in Data Block 7. The five elements found in aluminum alloy 6161, with the exception of zinc, were included in order to account for the light elements in the fuel plate cladding and end plates. The masses were calculated using only the active fuel length of each assembly, omitting the end boxes.

Data Blocks 11-15. These data blocks are used for entering data for the cask analysis portion of the SAS2H sequence. They may be omitted from the input file when the SKIPSHIPDATA parameter is included in Data Block 1.

Data Block 16. This block terminates the case input data. It consists of the keyword END in column one of the input file.

Program Execution

After an input file is created, the SAS2H module is executed by invoking the SCALE system driver. Appendix C contains one of the input files used in the analysis. The format for execution is:

SCALE4 INPUTFILENAME OUTPUTFILENAME

Multiple cases can be run sequentially by creating a DOS batch file using the following format for each case:

CALL SCALE4 INPUTFILENAME OUTPUTFILENAME

The SAS2H sequence was executed on three different PC systems to evaluate the code execution times. The first system was a Gateway P5-166XL with a 166MHz Pentium processor, 32MB EDO ram, and 2.2GB EIDE hard disk operated under Windows 95 (System A). The second system was an HP Vectra 6/XU with two 200MHZ Pentium Pro processors, 196MB of ECC ram, and 2GB Ultra-SCSI hard disk operated under Windows NT 4.0 (System B). The last system was a Dell Dimension XPS Pro200n with a 200MHz Pentium Pro processor, 64MB of ECC ram, and 4GB SCSI Ultra-Wide hard disk operated under Windows NT 4.0 (System C). A ten cycle (single library per cycle) power history case was evaluated by each system. Table V-1 lists the program execution times. It appears that hard disk access time has a significant impact on run-time because temporary files on the hard drive are accessed each time the output file of one module is used to create the input file for a subsequent module.

Table V-1: System Run-Time Comparison

SYSTEM	RUN-TIME (s)
A	2612
B	1109
C	970

Model Analysis.

The models could not be validated in the same manner as the validations that were presented in Chapter II because of the inability to perform an isotopic analysis on the reactor fuel. Alternatively a study of the effects of the larger unit cell design, composition temperature, fuel loading and power history on spent fuel predictions was performed. A model comparison was conducted to determine the impact of varying the larger unit cells. The same power history was applied to five different models representing full, control, and core-average fuel assemblies. The composition temperatures were then lowered to determine the effect on the output. A power history comparison was then used to determine the ability of ORIGEN-S to distinguish spent fuel produced under varying operating conditions. Seven different power histories, each representing the total nine years of core operation, were applied to a standard fuel assembly model. The results of these comparisons are presented in the following chapters.

Description of Output.

The user can adjust the detail of the SAS2H output by specifying the PRINTLEVEL parameter. PRINTLEVEL ranges from 1 (sparse) to 10

(verbose). Each functional code of the module has its own format and all output is directed to a single output file that is designated when the module is called. The size of the output files averaged over 5MB when using a PRINTLEVEL=5. The analysis was performed on data taken from the final depletion analysis output produced by the ORIGEN-S module. The isotopic concentrations of light element, actinides and fission products were calculated in grams. The assembly-averaged fluxes from each case were also compared. Appendix D contains an excerpt from the output produced during the final ORIGEN-S depletion case.

VI. Model Comparison

Overview.

This chapter investigates the effects of varying the design parameters that are used to create the input files. The first part of the comparison focused on the total fuel loading and larger unit cells of the models. The second part of the comparison studied the effects of varying the composition temperatures.

Total Fuel Loading/Larger Unit Cell Comparison.

Model Description. Six different models were designed to represent full and control fuel assemblies. Each model contained the same power history. The power history consisted of nine cycles, each representing the reactor's power production for a year represented by a single irradiation period at 500KW followed by a decay period for the remainder of the year.

Three models (1-3) were designed to represent a standard fuel assembly each using a different larger unit cell. Model 1 incorporates the standard fuel assembly cell, model 2 uses the core average cell based on 250KW operation, and model 3 is based on the core average-500KW cell. The remaining models (4-6) represent control fuel assemblies using the control fuel assembly cell (model 4), core average-250KW cell (model 5), and the core average-500KW cell (model 6).

The major differences between the cells are that core average cells contain the control rod mixture zones while the standard and control fuel assembly cells omit them. Additionally the 250KW and 500KW core average cells differ in the areas of control rod mixtures within the larger unit cells. The control rods are withdrawn further from the active fuel area during high power operation (500KW) than average power operation (250KW). This results in smaller areas of control rod mixtures (MX 4 and MX5) in the 500KW cell when compared to the 250KW cell.

The total fuel volume (VOLFUELTOT) and power (MW) per assembly (POWER) of the control fuel assembly models (4-6) is lower than the standard fuel assembly models (1-3) due to the removal of six fuel plates to accommodate the control rods.

Results: The final ORIGEN-S depletion analysis of the models calculated concentrations of 201 nuclides (25 light elements, 11 actinides, and 165 fission products) in the spent fuel. The output was analyzed by comparing average fluxes, variations in nuclide concentrations, and ratios of actinide concentrations.

The results of the average flux comparison are presented in Figure VI-1. ORIGEN calculates an assembly space-time-spectrum averaged flux using Equation (5) and the procedure described in chapter II. The ORIGEN average flux calculation does not provide significant meaningful information because spatial and spectrum effects are combined by the averaging process.

However the average flux was useful for evaluating the effects caused by varying the model design parameters. Each model should have produced an identical average flux because the power per assembly was scaled to fuel loading. The variation in average fluxes is caused by the differences in deriving cross sections from different larger unit cell models. The standard fuel assembly larger unit cell used in model 1 did not include the inner moderator zone found in the other larger unit cells. The lack of additional moderator results in a flux spectrum that is higher energy weighted, produces the lowest fission cross sections, and requires the highest average flux to produce equivalent power. Model 4 includes the inner moderator zone but does not incorporate the control rod zones. This model required the lowest average flux because it produces the highest fission cross sections. Models 2, 3, 5 and 6 produced nearly identical average flux calculations because all used the same core average-250KW cell. The inclusion of the control rod zones in the core average-250KW cell requires a higher average flux than model 4. The variations in the calculated average flux illustrate the changes in cross section calculation caused by varying the larger unit cell design.
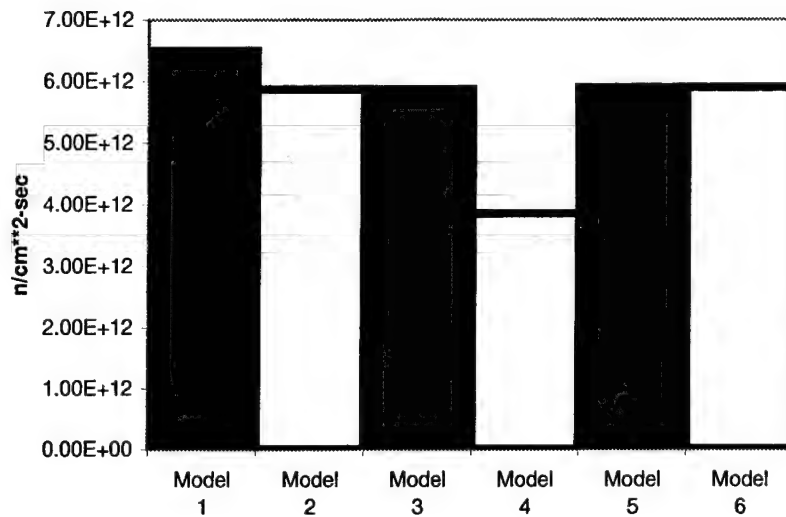
Figure VI-1: Model Comparison Average Fluxes

The next part of the comparison focused on the compositions of the spent fuel. Actinide concentration ratios were examined (Figure VI-2 through Figure VI-7) and inconsistencies in nuclide concentrations were identified (Figure VI-8). The models produced nearly identical concentrations for the majority of the nuclides.
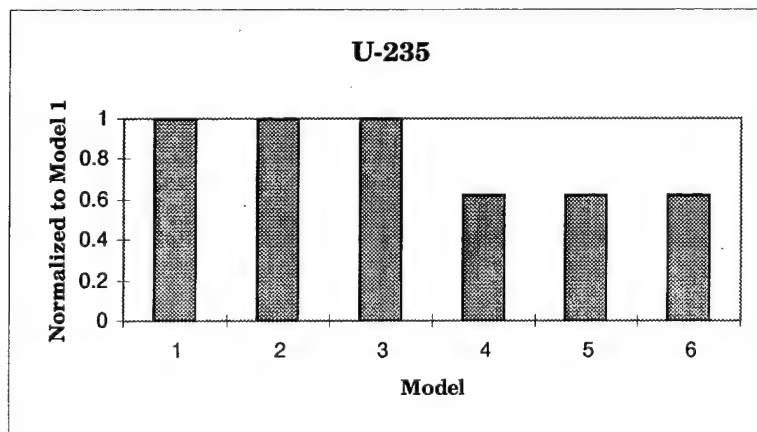
Figure VI-2: ^{235}U Model Comparison
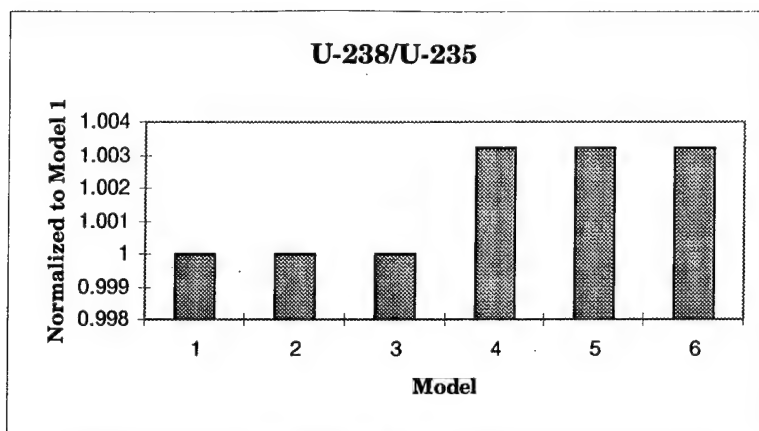
Figure VI-3: $^{238}U/^{235}U$ **Model Comparison**
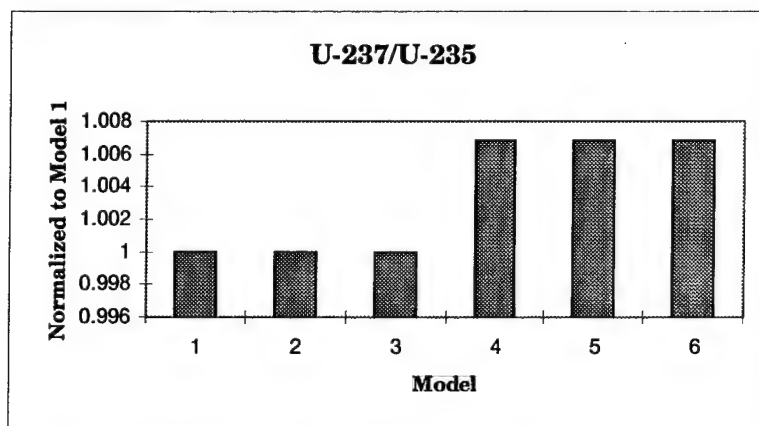
Figure VI-4: $^{237}U/^{235}U$ **Model Comparison**
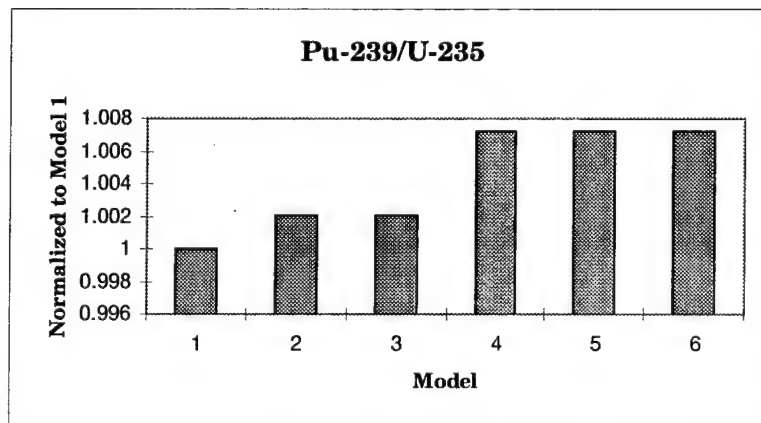
Figure VI-5: $^{239}Pu/^{235}U$ **Model Comparison**
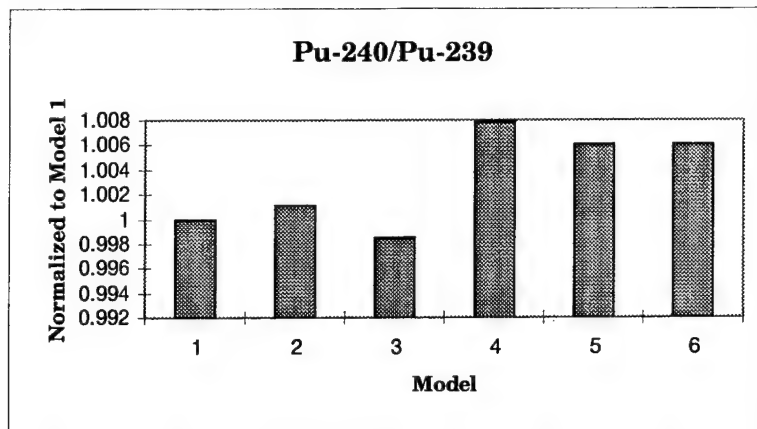
Figure VI-6: ^{240}Pu/^{239}Pu Model Comparison
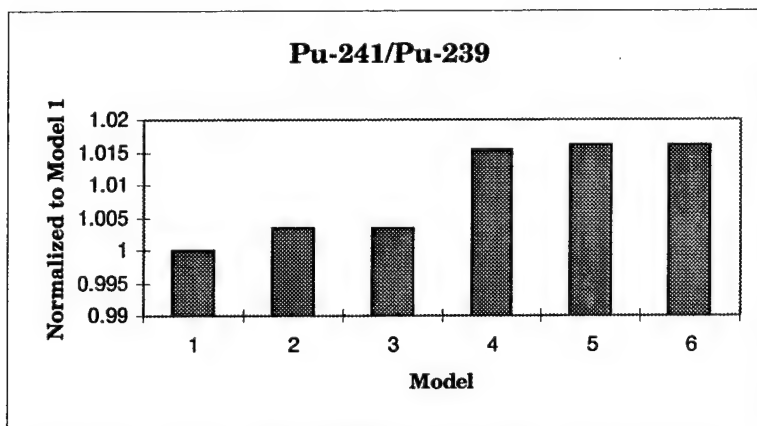
Figure VI-7: ^{241}Pu/^{239}Pu Model Comparison
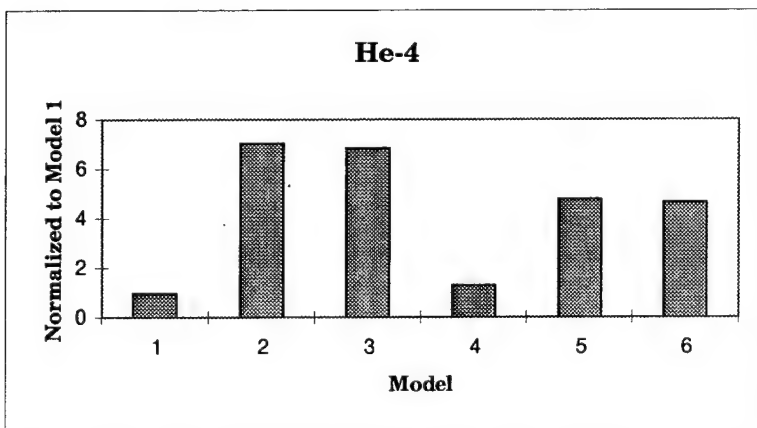
Figure VI-8: ^{4}He Model Comparison

The amount (grams) of each nuclide per assembly was calculated and compared. Note that the concentrations are for the total assembly, it is not possible to isolate the fuel or any other region of the larger unit cell. Three types of variations were observed during the composition analysis: variations due to differences in fuel loading, variations due to larger unit cell design, and variations due to a combination of different fuel loading and unit cell. The amount of ^{235}U and ratios of the other uranium nuclides to it (Figure VI-2 – Figure VI-4) are examples of variations induced by differences in model fuel loading. Figure VI-2 does not imply that the control fuel assemblies depleted 40% of their fuel, but indicates the difference in initial fuel loading caused by the removal of the six inner fuel plates. This type of variation is characterized by nearly identical results among model types: standard fuel assembly (models 1-3) and control rod fuel assembly (models 4-6). Concentrations of ^{4}He (Figure VI-8) provide an example of variations prompted by differences in cell design. The higher concentrations that were produced by the models based on the core average cells are due to the inclusion of the control rods in the larger unit cells. The boron in the safety rods increased helium production by neutron absorption ($_6B^{11} + _0n^1 \rightarrow 3\ _2He^4$). The plutonium concentration ratios (Figure VI-5 through Figure VI-7) provide examples of the last type of variation. There are significant differences between model types (standard assembly and control assembly) and smaller variations among the types caused by differences in cell design.

The magnitudes of the variations in actinide concentrations (<2%) were much smaller than the uncertainties (3-20%) derived from the validation studies discussed in Chapter II. This indicates that the concerns of properly designing the larger unit cell were unfounded because the variations due to model design are insignificant when compared to the validated accuracy of the code.

A single cell design was needed to evaluate the impact of varying the composition temperatures and power history. The standard assembly cell and control fuel assembly cells were not selected because they omit the control rods. The core average-250KW cell was chosen because it best represents the research reactor operating under average conditions.

Composition Temperature Comparison.

Model Description. Two models, each representing standard fuel assemblies, were compared by varying their composition temperatures. Both models were based on the core average-250KW cell. One model (Max) represents the reactor operating at its maximum power level of 500KW using the composition temperature discussed in the previous chapter. The other model (Min) represents the lowest temperature extreme, corresponding to a cold startup temperature. All composition temperatures in model-Min were specified to be the coolant inlet temperature of 296K. The power history used above, to compare the larger unit cells, was applied to both of these models.

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These models represent the extremes of the research reactor operating temperatures.

Results. The output was analyzed using the same method used to compare the fuel loading and unit cells. Once again the majority of the nuclide concentrations were nearly identical. Slight variations were observed in the actinides (Figure VII-9) and light elements (Figure VII-10). Higher concentrations of actinides in the maximum temperature model are a result of the Doppler broadening of the resonance neutron absorption cross sections of ^{238}U resulting from the higher composition temperatures. Similarly, the light elements have a higher resonance neutron absorption cross section at the highest temperature and result in lower concentrations in the maximum temperature model.

ACTINIDE CONCENTRATIONS
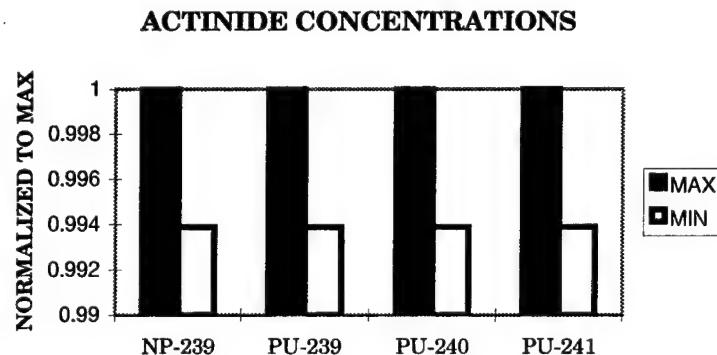
Figure VI-9: Actinide Temperature Comparison

LIGHT ELEMENT CONCENTRATIONS
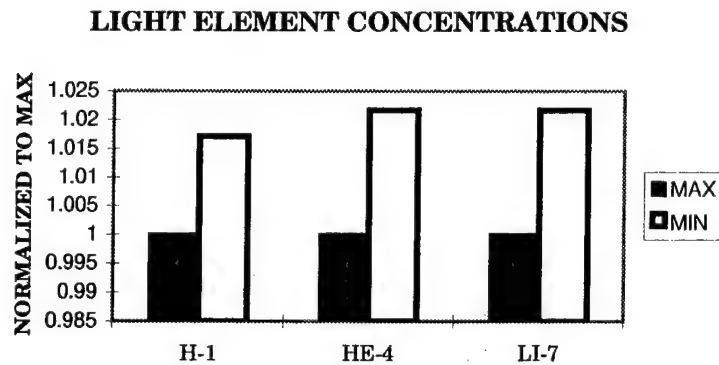
Figure VI-10: Light Element Temperature Comparison

Analysis.

The results of the comparison of the example problem data indicate that the design parameters (fuel loading, cell design, and composition temperatures) of the reactor model will affect the average flux and spent fuel isotopics. However, the variations observed were rather slight when compared with the uncertainties derived from the validation studies. The magnitude of the variations may be due to the size of the research reactor and its limited operating range. Models of reactors with larger operating ranges may produce results with larger variations by changing the model design parameters. A similar analysis should be applied to a larger system to determine if the impact of the model design parameters is insignificant when compared to the validation uncertainties. The constraint of a single temperature specification for each composition is also a potential limitation

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when attempting to model a reactor operating under a variety of temperature conditions.

VII. Power History Comparison

Overview.

This chapter presents the comparison that was used to investigate the impact of varying the model power history. The SAS2H limitation of 25 cycles prevented an exact representation of the OSURR power history. At least 150 cycles per year would be needed to model the daily operation schedule of the reactor. Seven different variations of the total nine-year power history were applied to a model using the core average-250KW cell to assess the impact of power history on the output.

Power History Description.

The historical data that was available from the research reactor listed each year's operation in megawatt-hours (Table VII-1). This data was then used to create seven distinct power histories that each represent the same total power production. Each history ended with an identical final cycle consisting of 6 hours of 250KW operation followed by a 24-hour decay period. The identical last cycle was used to minimize the differences due to short-lived nuclides. The number of cycles per history varied from a minimum of 2 to the maximum of 25. Each cycle specifies the power per assembly (POWER) in megawatts, length of irradiation period (BURN) in days, and length of zero power period (DOWN) also in days. The seven power histories are detailed in Tables VII-1 through VII-3. The histories differ in the number

of cycles used to recreate the nine years of operation of the research reactor. The other significant difference among the power histories is the reactor power level. The research reactor is operated under a variety of power levels based on the requirements of experiments.

Power histories were designed using low, average (250KW), and high (500KW) power levels. Cycle lengths varied from 22.8 days to 1 year with the exception of the last cycle that always represented 30 hours. The impact of combining yearly cycles with high power levels results in very short irradiation periods followed by very long decay periods. The 25 cycle power histories (2 and 5) were designed by modifying histories based on yearly cycles (1 and 4) by dividing the ninth year of operation into 22.8 day cycles in an effort to reduce the long decay periods near the end of the history. Two histories (3 and 7) were designed to eliminate all of the decay periods except for the final cycle by operating at very low power continuously. History 3 is based on a constant power level for all nine years while history 7 uses a yearly power level based on annual usage. History 6 was designed to reflect the actual operating routine of the research reactor. The reactor averages 52 days of operation per year. History 6 was created by dividing the reactor's yearly power production equally among 52 days and then representing it by two six-month cycles.

Table VII-1: Research Reactor Yearly Operation

Year	MW-h
88/89	0.723
89/90	1.152
90/91	2.035
91/92	21.424
92/93	30.056
93/94	21.405
94/95	160.220
95/96	83.640
96/97	102.950

Table VII-2: Power History (1,2,4) Data

CYCLE	History 1			History 2			History 4		
	POWER	BURN	DOWN	POWER	BURN	DOWN	POWER	BURN	DOWN
1	0.013	0.1204	364.8796	0.013	0.1204	364.8796	0.026	0.0602	364.9398
2	0.013	0.192	364.808	0.013	0.192	364.808	0.026	0.096	364.904
3	0.013	0.3392	364.6608	0.013	0.3392	364.6608	0.026	0.1696	364.8304
4	0.013	3.5684	361.4316	0.013	3.5684	361.4316	0.026	1.7842	363.2158
5	0.013	5.0092	359.9908	0.013	5.0092	359.9908	0.026	2.5046	362.4954
6	0.013	3.5676	361.4324	0.013	3.5676	361.4324	0.026	1.7838	363.2162
7	0.013	26.704	338.296	0.013	26.704	338.296	0.026	13.352	351.648
8	0.013	13.94	351.06	0.013	13.94	351.06	0.026	6.97	358.03
9	0.013	16.9084	346.8416	0.013	1.0724	21.7401	0.026	8.454	355.296
10	0.013	0.25	1	0.013	1.0724	21.7401	0.013	0.25	1
11				0.013	1.0724	21.7401			
12				0.013	1.0724	21.7401			
13				0.013	1.0724	21.7401			
14				0.013	1.0724	21.7401			
15				0.013	1.0724	21.7401			
16				0.013	1.0724	21.7401			
17				0.013	1.0724	21.7401			
18				0.013	1.0724	21.7401			
19				0.013	1.0724	21.7401			
20				0.013	1.0724	21.7401			
21				0.013	1.0724	21.7401			
22				0.013	1.0724	21.7401			
23				0.013	1.0724	21.7401			
24				0.013	0.8224	20.7401			
25				0.013	0.25	1			
	250KW			250KW			500KW		
	YEAR CYCLES			LAST YEAR 3WK CYCLES			YEAR CYCLES		

Table VII-3: Power History (3) Data

		History 3	
CYCLE	POWER	BURN	DOWN
1	0.000279	3283.75	0
2	0.013	0.25	1
	10.73KW STEADY POWER		

Table VII-4: Power History (5-7) Data

		History 5			History 6			History 7	
CYCLE	POWER	BURN	DOWN	POWER	BURN	DOWN	POWER	BURN	DOWN
1	0.026	0.0602	364.9398	0.000013	26	156.5	4.29E-06	365	0
2	0.026	0.096	364.904	0.000013	26	156.5	6.84E-06	365	0
3	0.026	0.1696	364.8304	0.000048	26	156.5	1.21E-05	365	0
4	0.026	1.7842	363.2158	0.000048	26	156.5	0.000127	365	0
5	0.026	2.5046	362.4954	8.48E-05	26	156.5	0.000178	365	0
6	0.026	1.7838	363.2162	8.48E-05	26	156.5	0.000127	365	0
7	0.026	13.352	351.648	0.000892	26	156.5	0.000951	365	0
8	0.026	6.97	358.03	0.000892	26	156.5	0.000496	365	0
9	0.026	0.544	22.2685	0.001252	26	156.5	0.000604	363.75	0
10	0.026	0.544	22.2685	0.001252	26	156.5	0.013	0.25	1
11	0.026	0.544	22.2685	0.000892	26	156.5			
12	0.026	0.544	22.2685	0.000892	26	156.5			
13	0.026	0.544	22.2685	0.006676	26	156.5			
14	0.026	0.544	22.2685	0.006676	26	156.5			
15	0.026	0.544	22.2685	0.003485	26	156.5			
16	0.026	0.544	22.2685	0.003485	26	156.5			
17	0.026	0.544	22.2685	0.004227	26	156.5			
18	0.026	0.544	22.2685	0.004227	26	155.25			
19	0.026	0.544	22.2685	0.013	0.25	1			
20	0.026	0.544	22.2685						
21	0.026	0.544	22.2685						
22	0.026	0.544	22.2685						
23	0.026	0.544	22.2685						
24	0.026	0.294	21.19038						
25	0.013	0.25	1						
	500KW 1YR CYCLES			52 BURN DAYS/YR			STEADY POWER		
	LAST YR 22.8125 DAY/CYCLE			2 CYCLES/YR			YEAR CYCLES		

Results.

The power histories were compared in the same manner as the models.

The fluxes that ORIGEN-S calculated (Figure VII-1) were as expected,

varying proportionally with power level. Analysis of the compositions of the

spent fuel again resulted in several observations. Once again the majority of

the 201 nuclide concentrations, including ^{235}U and ^{238}U, were nearly

identical. Figure VII-2 illustrates the discrepancy in ^{237}U concentration. The

absences are due to the short half-life (6.75 days) of ^{237}U combined with the

long decay periods present in histories 1, 4, and 6.
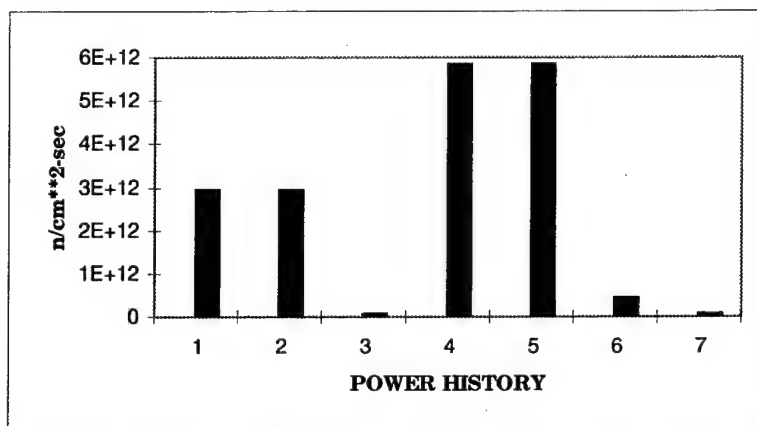
Figure VII-1: Power History Comparison Average Fluxes
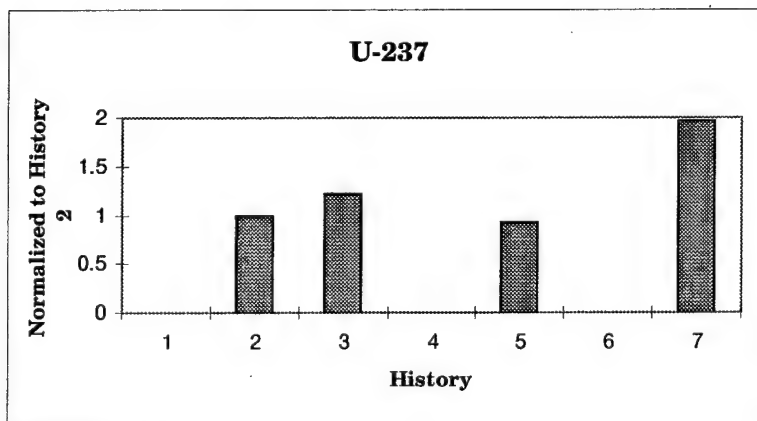
VII-2: ^{237}U Power History Comparison

Variations in the actinide concentration ratios (Figure VII-3 through

Figure VII-7) and inconsistencies in light element concentrations (Figure VII-

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8 through Figure VII-13) were also identified.
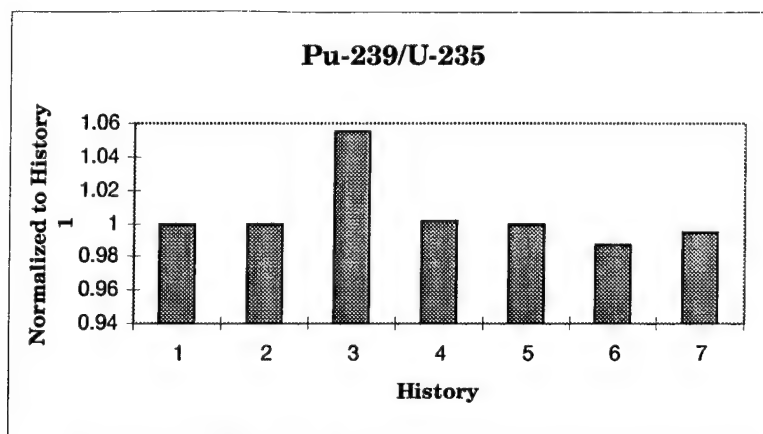
Figure VII-3: ^{239}Pu/^{235}U Power History Comparison
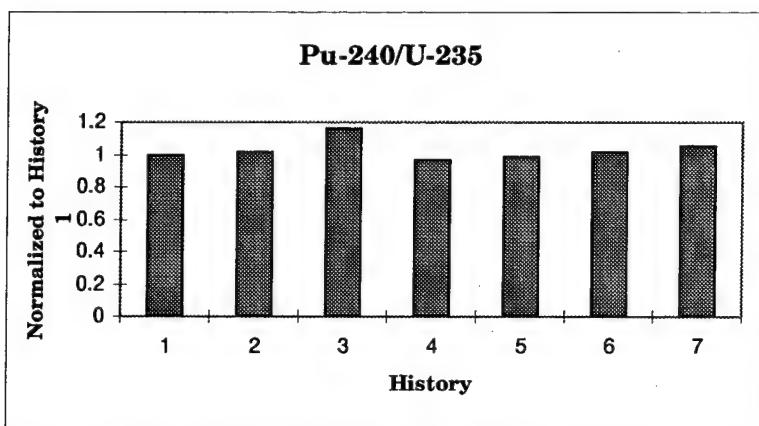
Figure VII-4: ^{240}Pu/^{235}U Power History Comparison
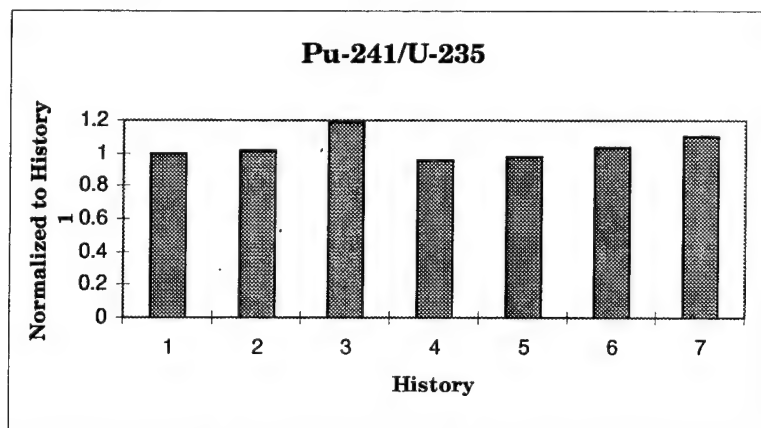
Figure VII-5: ^{241}Pu/^{235}U Power History Comparison
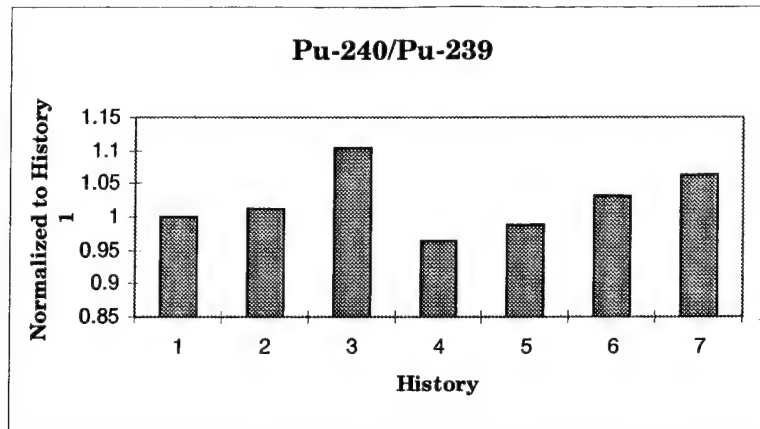
Figure VII-6: ^{240}Pu/^{239}Pu Power History Comparison
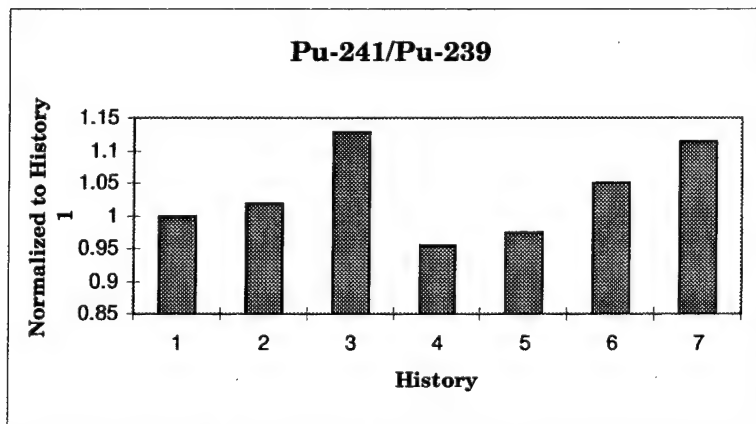
Figure VII-7: ^{241}Pu/^{239}Pu Power History Comparison
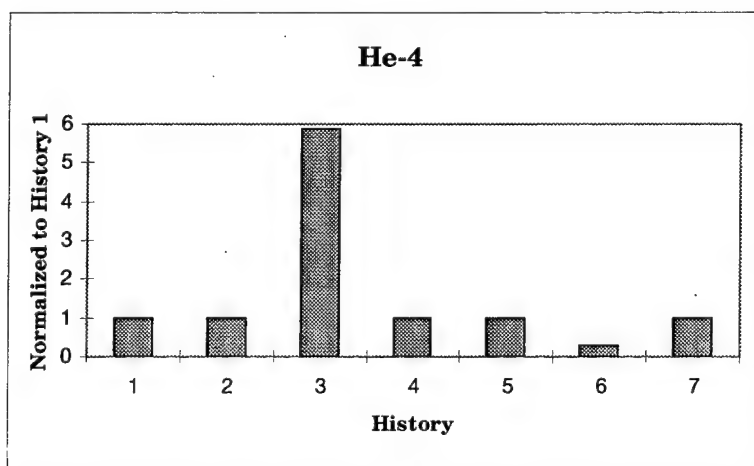
Figure VII-8: ^{4}He Power History Comparison
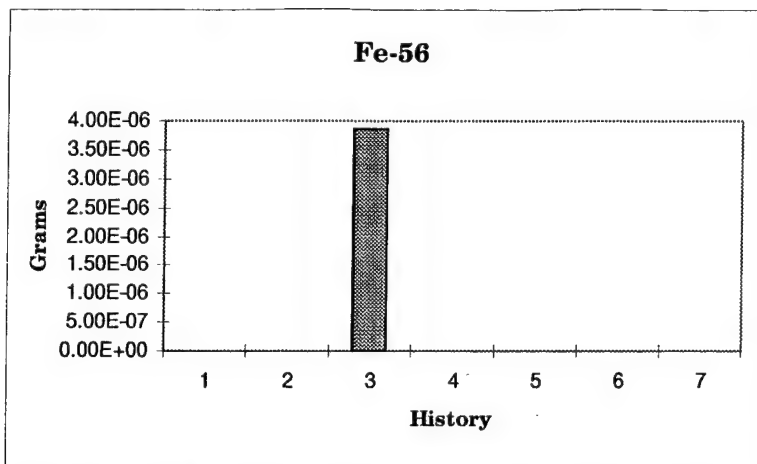
Figure VII-9: ^{56}Fe Power History Comparison
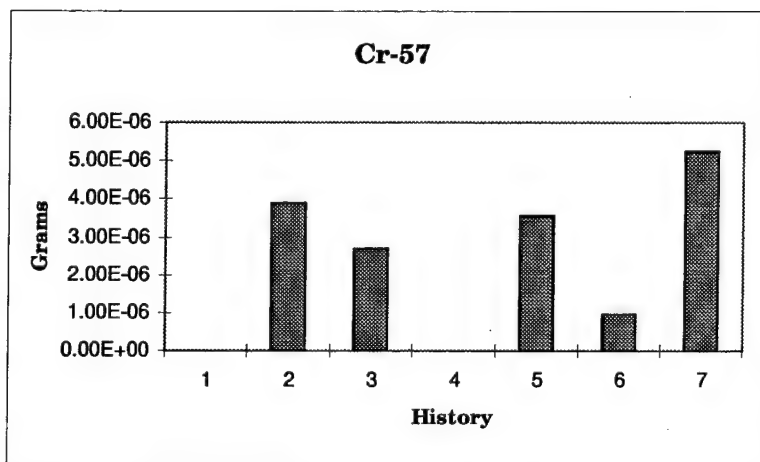
Figure VII-10: ^{57}Cr Power History Comparison
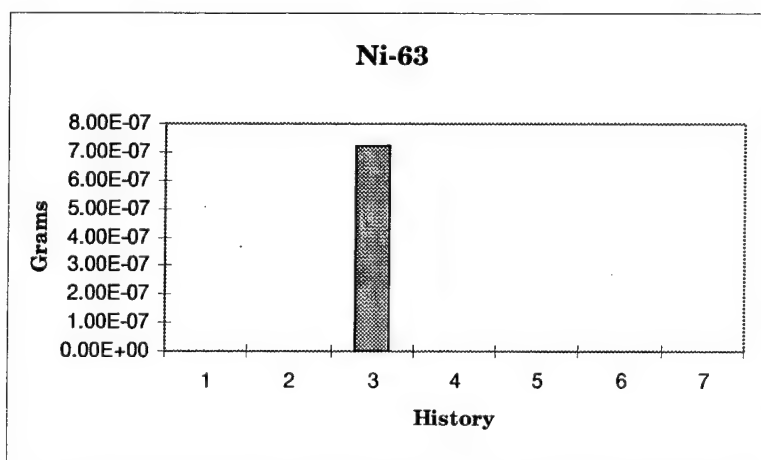
Figure VII-11: ^{63}Ni Power History Comparison

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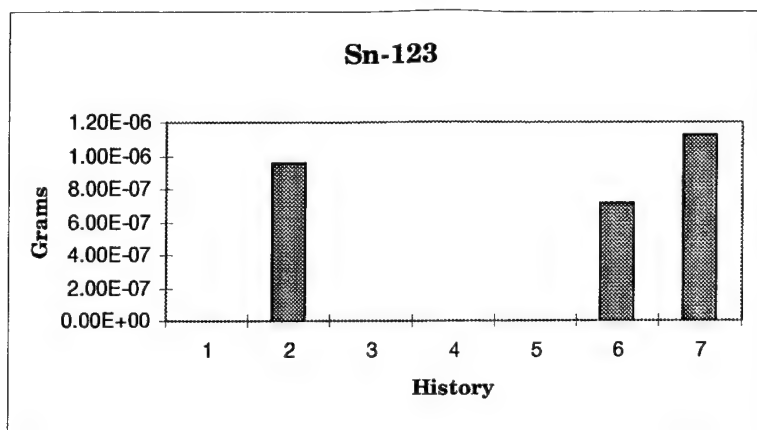
Figure VII-12: ^{123}Sn Power History Comparison
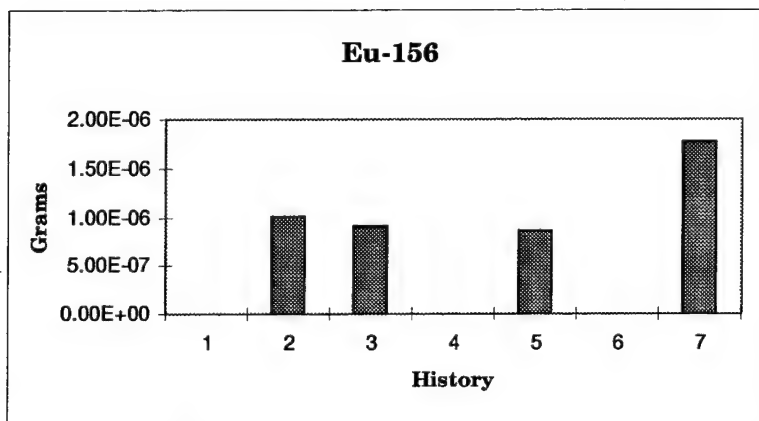
Figure VII-13: ^{156}Eu Power History Comparison

The increased concentrations of plutonium (Figure VII-3 through

Figure VII-7) and helium (Figure VII-8) resulting from history 3 are a result

of an inconsistency in the average flux. When the average flux of history 3 is

integrated over the total irradiation time the resulting neutron fluence is

higher than the fluence produced by the other power histories. The increased

neutron fluence leads to an increase in resonance neutron absorption by ^{238}U

and ^{11}B. The inconsistency in the average flux is probably due to the use of

only two cycles to represent history 3 while the other histories were comprised of at least ten cycles. The last observation was that several isotopes were identified (Figure VII-9 through Figure VII-13) at very low concentrations (10^{-7}-10^{-6} g) in only specific histories, with the remainder of the histories predicting concentration below the code's threshold ($\sim10^{-7}$ g).

Analysis.

This comparison demonstrates the capability of ORIGEN-S to distinguish spent fuel produced under varying reactor-operating conditions. The variations in nuclide concentrations due to power history changes were more pronounced than the variations produced by changing the other model design parameters. This indicates that the power history specification may be the most important design parameter when considering the effect on output. The limitation of 25-cycles may not be a constraint when modeling commercial power reactors that typically operate on 12-18 month refueling cycles. It does however limit the accuracy of modeling a system like the research reactor that operates on a non-routine schedule. The magnitude of the variations observed in the example case may be due to the limited power range of the research reactor. I would expect much greater variations from a larger system with greater power operating range.

VIII. Conclusions

Applications

These model-creating methodologies can be used to create reactor-specific cross-section libraries for the ORIGEN2 and ORIGEN-S codes when the generic models provided with the codes are inadequate. ORIGEN can be used in the classification of spent nuclear fuel by providing a prediction of isotopic composition that can be compared to results of a chemical analysis.

The speed and flexibility of ORIGEN-S make it the preferred method. While it lacks the multidimensional analysis that is included in preparing ORIGEN2 libraries, ORIGEN-S can rapidly produce new models using significantly fewer computational resources with a single software package. The SCALE4.3 system allows the user to create and execute new ORIGEN-S models on either a PC or UNIX system. There are situations when the use of ORIGEN2 would be preferred over ORIGEN-S. Systems that have significant axial variation would not be adequately represented by the 1-D calculations used to create the ORIGEN-S libraries. Another instance where the computational effort of creating a new ORIGEN2 library would be justified would be the creation of a model that would be used routinely.

Limitations

Both methodologies require detailed data (initial isotopics, dimensions, geometry, operating temperatures, power history) about the system to be

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modeled. The accuracy of the results of the codes is also highly dependent on the quality of the neutronics data that is provided to them. It is also important to emphasize that the codes will predict assembly-averaged compositions. The following sections address the individual limitations of the codes.

SAS2H/ORIGEN-S. The most significant limitation of SAS2H is the use of 1-D computations to derive the neutronics data. This limits the ability to model systems having large axial variations. The results of SAS2H are also dependent on the design parameters used to define the reactor models. This research indicates that the larger unit cell design, and composition temperature will have a minor impact on the output, while the power history has greater impact on the results. The ability to create models that produce consistent, accurate results will require the user to master the art of design parameter specification. Additionally, the sequence assumes a single fuel-pin unit-cell (all assembly pins are assumed to have a constant enrichment and pitch); this complicates the analysis of systems composed of widely varying fuel elements. The code also assumes that the temperatures applied to each zone of the unit cell are constant. Large systems that have significant spatial variation in temperature, and systems operated under varying temperature conditions will not generate accurate results.

ORIGEN2. The most significant limitation involved with the creation of new ORIGEN2 cross section libraries is the lack of an integrated code package to perform the necessary calculations. The user must perform the multidimensional depletion calculations to generate the burnup dependent cross sections and flux parameters and then convert the data into ORIGEN2-compatible libraries. The process is significantly more resource intensive than ORIGEN-S.

Recommendations.

AFTAC should consider the use of ORIGEN as a potential resource for the classification of spent nuclear fuel. ORIGEN provides the ability to generate calculated isotopic predictions that can be used for comparison with experimental measurements. The SCALE system is a single software package that allows the user to rapidly generate new ORIGEN models on a PC.

The next step in this research should be the application of this method to a system with known isotopics, preferably a system with a significantly higher burnup than the OSU reactor. The total burnup of the research reactor, approximately 900MWD/T, is significantly lower than the 20000-30000 MWD/T burnup of a typical commercial PWR. Modeling a larger system would confirm or deny the indication that the variations induced by varying the design parameters are insignificant when compared to the uncertainty of the code, regardless of the size of the reactor. This would

provide a proper validation and provide further insight into the model design process by developing techniques for the proper selection of model design parameters. Another area that deserves attention is a comparison of the automatic rapid processing methodology with the standard SAS2H sequence. Another method of decreasing program execution time may be explored by recompiling and rebuilding the SCALE executable files. The current executable files use a DOS extender. Rebuilding the executables utilizing current flat-memory-model compilers may significantly improve program execution times. A comparison of results derived from one- and multidimensional calculations by a direct comparison of ORIGEN2 and ORIGEN-S models may also be beneficial. Additionally there may be differences in deriving models with codes based on diffusion theory instead of codes based on transport theory. Lastly, consideration should be given to the development of a software package that would simplify the process of creating new cross section libraries for ORIGEN2. RSICC recently announced the availability of MOCUP, a utility developed at the Idaho National Engineering Laboratory to couple MCNP4A, a Monte Carlo based multidimensional transport code developed by Los Alamos National Laboratory, with ORIGEN2.1. This utility appears to have the potential to simplify the creation of new ORIGEN2 models.

Appendix A: SAS2 Input Data Requirements

This appendix contains information from Table S2.5.1 from the SAS2H

users manual (Hermann and Parks,1997:S2.5.3-8).

Data Block	Name or Keyword	Definition, comments, and examples
1	=SAS2*	(or =SAS2H as an alias name) Module activator, column 1.
2	TITLE	An 80-character title.
3	LIB	Name of SCALE library to be used in reactor analysis: 44GROUPNDF5 (recommended); 27BURNUPLIB (next alternative); 27GROUPNDF4; 238GROUPNDF5; HANSEN-ROACH; or for any other name the code uses library on unit number 70.
	GE	Reactor lattice type. SAS2 always requires LATTICECELL Example: 44GROUPNDF5 LATTICECELL
4	SC	Component name from Standard Composition Library
	MX	Mixture number of SC. MX≤3 if pin-cell; MX≥4 if cask or larger unit-cell mixture
	DEN=*	Density of the standard composition (optional), g/cm³
	VF	Density multiplier. Set to zero if using ADEN. May omit if END is next (1).
	ADEN	Atom density, atoms/barn-cm. Enter only if VF=0
	TEMP	Temperature, K, applied only if MX≤3 or if larger unit-cell mixture. May omit if END is next (293)
	IZA	SCALE ZA number. Omit if VF=0. Use only for multiple isotope elements.
	WTP	Wt% for IZA. Repeat IZA-WTP pairs for 100% sum.
	END*	End of this SC data. Repeat for all SC of case. Examples: FE 4 0 4.2 -3 END SS3044 6 END
	END COMP*	Ends entire material data input.

Data Block	Name or Keyword	Definition, comments, and examples
	CPT	Type of fuel lattice: SQUAREPITCH, TRIANGPITCH, or SYMMSLABCELL only allowed in SAS2
	PITCH	Center-to-center spacing between fuel pins or fuel slabs, cm
	FUELOD	Outside diameter of fuel in pin or fuel thickness in slab, cm
	MFUEL	Mixture number of fuel. Always enter 1 in SAS2
	MMOD	Moderator mixture number. Always enter 3 in SAS2
5	CLADOD	Clad outside diameter of rod or distance between outer clad surfaces of slab, cm. There must be SC for clad.
	MCLAD	Clad mixture number. Always 2 in SAS2
	CLADID	Clad inside diameter of rod or distance between inner clad surfaces of slab, cm. Omit this and next entry if no gap.
	MGAP	Gap mixture number, if gap. Always 0 in SAS2
	END*	End of reactor-lattice.
		Example: SQUAREPITCH 1.5 0.94 1 3 1.06 2 END
	MORE DATA*	Optional data for XSDRNPM cases run during depletion analysis. Entries may be in any order.
	SZF=*	Spatial mesh factor. SZF:<1 for finer; >1 for coarser mesh (1)
	ISN=*	Order of angular quadrature (8)
6	IIM=*	Maximum number of inner iterations (20)
	ICM=*	Maximum number of outer iterations (25)
	EPS=*	Overall convergence criteria (0.0001)
	PTC=*	Scalar flux point convergence (0.0001)
	IUS=*	IUS=:1, upscatter scaling to speed convergence; 0, not scaled (0)
	END*	End of option
		Example: MORE DATA ISN=16 SZF=0.9 END

Data Block	Name or Keyword	Definition, comments, and examples
	NPIN/ASSM=*	Number of fuel-rods/assembly; control rods not included; burnable-poison fuel rods included
	FUELNGTH=*	Active length of fuel in rods, cm
	NCYCLES=*	Number of cycles exposed; commonly number of years (3)
	NLIB/CYC=*	Number of libraries made per cycle (1)
	LIGHTEL=*	Number of light elements in clad and assembly input in Data Block 10
	PRINTLEVEL=*	Print level (integer) requested
	VOLFUELTOT=*	Total volume of the fuel (MX=1) in the entire assembly or quantity to which POWER applies, cm³. Always applied if non-zero. Do not enter for cylindrical fuel rods. Always enter for slab-lattice
	INPLEVEL=*	Input level of data below (0)
	NUMHOLES=*	Number of second type pins or "holes"/assembly. Required only if INPLEVEL=1
	NUMINSTR=*	Number of instrument tubes/assembly (1). Required only if INPLEVEL=1
	MXTUBE=*	Mixture number of guide tube (2). Required only if INPLEVEL=1
7	ORTUBE=*	Outside radius of guide tube, cm. Required only if INPLEVEL=1
	SRTUBE=*	Inside (small) radius of guide tube, cm. Required only if INPLEVEL=1
	ASMPITCH=*	Pitch between assemblies, cm. Required only if INPLEVEL=1
	NUMZTOTAL=*	Number of zones in describing larger cell. Required only if INPLEVEL=2 or 3
	MXREPEATS=*	=0/1; MIXES and RADIOUS required: for each library made/only once (1). Required only if INPLEVEL=2 or 3
	MIXMOD=*	Mixture number of moderator (3). Required only if INPLEVEL=2 or 3
	BPRNUM=*	Array data of number of burnable poison rods (BPRs) per assembly for each library segment of the NCYCLES*NLIB/CYC libraries. (First entry applies to first segment of first cycle, etc.) Not required if no BPRs or if all guide tubes contain BPRs. Never required unless INPLEVEL=2 or 3

Data Block	Name or Keyword	Definition, comments, and examples
	GTHOLENUM=*	Number of guide tubes without BPRs per assembly in first cycle of case. The number of guide tubes without BPRs for the remaining cycles is known implicitly by the total number of guide tubes minus BPRNUM. May include if BPRNUM is input or let code compute it. Never required unless INPLEVEL=2 or 3
7	FACMESH=*	Mesh size factor: Interval size=(default size)(FACMESH) is applied (1.0). Required if INPLEVEL=2 or 3
	LIMITGEO=*	Upper limit to the number of geometry intervals, after the default interval sizes and FACMESH are applied. If this value is exceeded, FACMESH is increased to where LIMITGEO is not exceeded (200). Required only if INPLEVEL=2 or 3
	END*	End of INPLEVEL scalar constants, required if INPLEVEL>0

(Repeat the following, as pairs of data, NUMZTOTAL times.)

(Enter NCYCLES*NLIB/CYC times if MXREPEATS=0)

Data Block	Name or Keyword	Definition, comments, and examples
8	MIXES	Mixture number of path-B zone, inner zone first. The next pair of data applies to the adjacent zone, etc. Use 500 for the fuel zone, composed of densities of the homogenized path-A unit cell computed by the code. Use mixture numbers 50 to 59, inclusive, for additional fuel zones. Required if INPLEVEL=2 or 3
	RADIUS	Outer radius of zone; ascending order, cm Example: 3 1.3 2 1.4 3 1.7 500 5.197

Data Block	Name or Keyword	Definition, comments, and examples
		Enter the following set for each cycle or NCYCLES times.
	POWER=*	Average power (megawatts) of either the assembly, an extended assembly increased to FUELNGTH, or the total fuel volume (if VOLFUELTOT>0.0)
	BURN=*	Fuel irradiation period of the reactor, d
9	DOWN=*	Downtime, d, following BURN; except for last cycle where it is cooling time of spent fuel used in cask analysis
	BFRAC=*	Fraction of first-cycle boron density (from Data Block 4) for this cycle (1)
	H2OFRAC=*	Fraction of first-cycle H_2O density for this cycle
	TEMKCYC	Temperature of all nuclides this cycle, K. Defaults to Standard Composition value
	END*	Required if any entry omitted
		Example: POWER=15.2 BURN=330 DOWN=35.25 END
		(Repeat the following LIGHTEL times, if LIGHTEL>0)
10	EL	Chemical symbol of element for which gamma source is to be included and (n, γ) Q-value/fission applied
	WTLITE	Effective weight/assembly, kg.
		Example: FE 6.2 CO 0.04 ZR 100
16	END*	End of SAS2 module data. Starts in column one. A new SCALE case may follow

*Word, words or name (including=), which must be part of data entry.

Values in parenthesis are default values.

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Appendix B: Fuel Plate Heat Transfer Analysis

A one-dimensional heat transfer analysis of the reactor fuel plates was conducted to determine the average temperatures of the fuel meat and cladding.

Under steady-state operating conditions, the amount of heat being generated in the nuclear fuel by fission is balanced by the removal of heat from the fuel to the cladding by conduction. Heat removal due to thermal conduction is proportional to the material thermal conductivity, k, and the temperature gradient. Equating the rate of energy production, S, to the rate of energy removal produces the following relation:

$$S = -\nabla \cdot k\nabla T. \tag{1}$$

Applying Equation (1) to the fuel region of a fuel plate (Figure B-1: Fuel Plate Half-Slab) results in the differential equation:

$$k_f u'' + S_f = 0. \tag{2}$$

When the additional conditions that the centerline fuel temperature is u_{CL} and the temperature gradient at the centerline, $u'(x)$ is zero are applied:

$$u(0) = u_{CL} \text{ and } u'(0) = 0,$$

a solution for the temperature in the fuel region results:

$$u(x)_{fuel} = \frac{2k_f u_{CL} - S_f x^2}{2k_f}. \tag{3}$$

Figure B-1: Fuel Plate Half-Slab
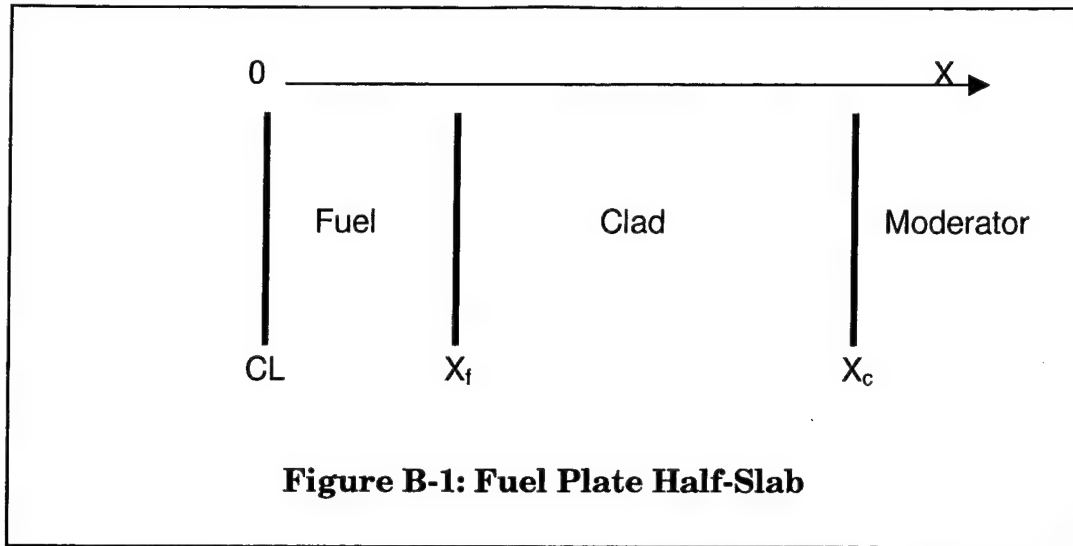
A similar solution for the clad region of the fuel plate can be determined by applying the conditions that the temperature, $u(x_f)$, and energy transfer at the fuel/clad interface be equal for both solutions:

$$u(x_f)_{clad} = u(x_f)_{fuel} \text{ and } k_{clad}\frac{du}{dx}\bigg|_{clad}(x_f) = k_{fuel}\frac{du}{dx}\bigg|_{fuel}(x_f),$$

producing the solution for the clad region:

$$u(x)_{clad} = \frac{k_{clad}(2k_{fuel}u_{CL} - S_f x_f) - k_{fuel}(x - x_f)(S_c(x - x_f) + 2S_f x_f)}{2k_{clad}k_{fuel}} \tag{4}$$

The Safety Analysis Report and Technical Specifications for the OSURR contains a heat transfer analysis that predicts the average clad surface temperature to be 56.5C (Ohio State University, 1987:110). The thermal conductivity of the cladding, k_{clad}, is167 W/m-K (ASM International, 1990:103). The thermal conductivity of the fuel was determined to be 159 W/m-K using Figure 8 of Appendix I, IAEA-TECDOC-643 (Matos and Snelgrove, 1992:I6.3). By substituting these values into Equation (4) the fuel

centerline temperature is calculated to be 56.57C. The fuel and cladding average temperatures where then determined to be 56.56C and 56.52C by integrating Equations (3) and (4) over the fuel and clad region respectively, yielding Equations (5) and (6).

$$\overline{u}_{fuel} = \frac{\displaystyle\int_0^{x_f} \frac{2k_f u_{CL} - S_f x^2}{2k_f} dx}{\displaystyle\int_0^{x_f} dx} \tag{5}$$

$$\overline{u}_{clad} = \frac{\displaystyle\int_{x_f}^{x_c} \frac{k_{clad}(2k_{fuel}u_{CL} - S_f x_f) - k_{fuel}(x - x_f)(S_c(x - x_f) + 2S_f x_f)}{2k_{clad}k_{fuel}} dx}{\displaystyle\int_{x_f}^{x_c} dx} \tag{6}$$

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Appendix C: Example Input File

```
=SAS2    PARM=(HALT10,SKIPSHIPDATA)
H7: OSURR- STEADY POWER ON YR CYCLES/FULL/AVG CELL 3-250
44GROUPNDF5  LATTICECELL

ARBMU3SI2AL 3.0 3 1 0 0 92000 22.01 14000 1.76 13027 76.23 1 1 329.56
92234 0.149 92235 19.5 92238 80.351 END
ARBMAL6161 2.7 8 1 0 0 13027 97.4 12000 1.0 14000 0.6 29000 0.3 24000 0.2
26000 0.35 25055 0.075 22000 0.075 2 1 329.53 END
H2O 3 325.3 END
SS304 4 325.3 END
ARBMSAFEROD 7.84 5 1 0 0 24304 19.0 25055 2.0 26304 67.5 28304 9.5
5000 1.5 5 1 325.3 END
END COMP

SYMMSLABCELL 0.417 0.051 1 3 0.127 2 END

NPIN/ASSM=16 FUELNGTH=60.96 NCYCLES=10 NLIB/CYC=1
PRINTLEVEL=5 LIGHTEL=5
VOLFUELTOT=303.36 INPLEVEL=2 NUMZTOTAL=7 END
3 .2762 4 .3133 5 .4655 3 1.1185 500 3.5304 2 3.9152 3 4.0570

POWER=0.00000429  BURN=365     DOWN=0     END
POWER=0.00000684  BURN=365     DOWN=0     END
POWER=0.0000121   BURN=365     DOWN=0     END
POWER=0.000127    BURN=365     DOWN=0     END
POWER=0.000178    BURN=365     DOWN=0     END
POWER=0.000127    BURN=365     DOWN=0     END
POWER=0.000951    BURN=365     DOWN=0     END
POWER=0.000496    BURN=365     DOWN=0     END
POWER=0.000604    BURN=363.75  DOWN=0     END
POWER=0.013       BURN=. 25    DOWN=1.    END

AL 2.8293 MG .0289 SI .01734 CU .00867 CR .00578
END
```

Appendix D: Example Output

H7: OSURR- STEADY POWER ON YR CYCLES/FULL/AVG CELL 3-250
LIGHT ELEMENTS   PAGE 51
DECAY, FOLLOWING REACTOR IRRADIATION IDENTIFIED BY: POWER= 2.793E-04MW, BURNUP=9.1727E-01MWD, FLUX= 6.31E+10N/CM**2-SEC

NUCLIDE CONCENTRATIONS, GRAMS
BASIS =SINGLE REACTOR ASSEMBLY

	INITIAL	0.2 D	0.3 D	0.5 D	0.7 D	0.8 D	1.0 D
H 1	1.74E-06	1.74E-06	1.74E-06	1.74E-06	1.74E-06	1.74E-06	1.74E-06
HE 4	9.23E-06	9.23E-06	9.23E-06	9.23E-06	9.23E-06	9.23E-06	9.23E-06
LI 7	1.38E-05	1.38E-05	1.38E-05	1.38E-05	1.38E-05	1.38E-05	1.38E-05
B 10	5.68E-01	5.68E-01	5.68E-01	5.68E-01	5.68E-01	5.68E-01	5.68E-01
B 11	2.51E+00	2.51E+00	2.51E+00	2.51E+00	2.51E+00	2.51E+00	2.51E+00
MG 24	2.25E+01	2.25E+01	2.25E+01	2.25E+01	2.25E+01	2.25E+01	2.25E+01
MG 25	2.97E+00	2.97E+00	2.97E+00	2.97E+00	2.97E+00	2.97E+00	2.97E+00
MG 26	3.40E+00	3.40E+00	3.40E+00	3.40E+00	3.40E+00	3.40E+00	3.40E+00
AL 27	2.83E+03	2.83E+03	2.83E+03	2.83E+03	2.83E+03	2.83E+03	2.83E+03
SI 28	1.59E+01	1.59E+01	1.59E+01	1.59E+01	1.59E+01	1.59E+01	1.59E+01
SI 29	8.36E-01	8.36E-01	8.36E-01	8.36E-01	8.36E-01	8.36E-01	8.36E-01
SI 30	5.74E-01	5.74E-01	5.74E-01	5.74E-01	5.74E-01	5.74E-01	5.74E-01
P 31	2.85E-06	2.85E-06	2.85E-06	2.85E-06	2.86E-06	2.86E-06	2.86E-06
V 51	1.69E-04	1.69E-04	1.69E-04	1.69E-04	1.69E-04	1.69E-04	1.69E-04
CR 50	2.41E-01	2.41E-01	2.41E-01	2.41E-01	2.41E-01	2.41E-01	2.41E-01
CR 51	5.25E-06	5.23E-06	5.21E-06	5.18E-06	5.16E-06	5.14E-06	5.12E-06
CR 52	4.84E+00	4.84E+00	4.84E+00	4.84E+00	4.84E+00	4.84E+00	4.84E+00
CR 53	5.59E-01	5.59E-01	5.59E-01	5.59E-01	5.59E-01	5.59E-01	5.59E-01
CR 54	1.42E-01	1.42E-01	1.42E-01	1.42E-01	1.42E-01	1.42E-01	1.42E-01
MN 55	4.73E+00	4.73E+00	4.73E+00	4.73E+00	4.73E+00	4.73E+00	4.73E+00
NI 64	7.66E-04	7.67E-04	7.67E-04	7.67E-04	7.68E-04	7.68E-04	7.68E-04
CU 63	5.94E+00	5.94E+00	5.94E+00	5.94E+00	5.94E+00	5.94E+00	5.94E+00
CU 64	4.19E-06	3.37E-06	2.71E-06	2.18E-06	1.75E-06	1.41E-06	1.13E-06
CU 65	2.73E+00	2.73E+00	2.73E+00	2.73E+00	2.73E+00	2.73E+00	2.73E+00
ZN 64	4.52E-04	4.52E-04	4.52E-04	4.53E-04	4.53E-04	4.53E-04	4.53E-04
ZN 66	2.71E-04	2.71E-04	2.71E-04	2.71E-04	2.71E-04	2.71E-04	2.71E-04
TOTAL	2.90E+03	2.90E+03	2.90E+03	2.90E+03	2.90E+03	2.90E+03	2.90E+03

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DECAY, FOLLOWING REACTOR IRRADIATION IDENTIFIED BY: POWER= 2.793E-04MW, BURNUP=9.1727E-01MWD, FLUX= 6.31E+10N/CM**2-SEC

NUCLIDE CONCENTRATIONS, GRAMS
BASIS =SINGLE REACTOR ASSEMBLY

	INITIAL	0.2 D	0.3 D	0.5 D	0.7 D	0.8 D	1.0 D
TH230	7.42E-06	7.42E-06	7.42E-06	7.42E-06	7.42E-06	7.42E-06	7.42E-06
U234	2.97E-01	2.97E-01	2.97E-01	2.97E-01	2.97E-01	2.97E-01	2.97E-01
U235	3.79E+01	3.79E+01	3.79E+01	3.79E+01	3.79E+01	3.79E+01	3.79E+01
U236	1.71E-01	1.71E-01	1.71E-01	1.71E-01	1.71E-01	1.71E-01	1.71E-01
U237	2.06E-06	2.03E-06	1.99E-06	1.96E-06	1.92E-06	1.89E-06	1.86E-06
U238	1.61E+02	1.61E+02	1.61E+02	1.61E+02	1.61E+02	1.61E+02	1.61E+02
NP237	1.56E-04	1.56E-04	1.56E-04	1.56E-04	1.56E-04	1.56E-04	1.56E-04
NP239	2.89E-04	2.93E-04	2.79E-04	2.65E-04	2.53E-04	2.41E-04	2.29E-04
PU239	5.36E-02	5.36E-02	5.37E-02	5.37E-02	5.37E-02	5.37E-02	5.37E-02
PU240	4.22E-04	4.22E-04	4.22E-04	4.22E-04	4.22E-04	4.22E-04	4.22E-04
PU241	3.01E-06	3.01E-06	3.01E-06	3.01E-06	3.01E-06	3.01E-06	3.01E-06
TOTAL	1.99E+02	1.99E+02	1.99E+02	1.99E+02	1.99E+02	1.99E+02	1.99E+02

DECAY, FOLLOWING REACTOR IRRADIATION IDENTIFIED BY: POWER= 2.793E-04MW, BURNUP=9.1727E-01MWD, FLUX= 6.31E+10N/CM**2-SEC

NUCLIDE CONCENTRATIONS, GRAMS
BASIS =SINGLE REACTOR ASSEMBLY

	INITIAL	0.2 D	0.3 D	0.5 D	0.7 D	0.8 D	1.0 D
H 3	1.21E-06	1.21E-06	1.21E-06	1.21E-06	1.21E-06	1.21E-06	1.21E-06
AS 75	3.69E-06	3.69E-06	3.70E-06	3.70E-06	3.70E-06	3.70E-06	3.70E-06
GE 76	1.23E-05	1.23E-05	1.23E-05	1.23E-05	1.23E-05	1.23E-05	1.23E-05
SE 77	2.70E-05	2.70E-05	2.70E-05	2.70E-05	2.70E-05	2.70E-05	2.70E-05
SE 78	7.12E-05	7.13E-05	7.13E-05	7.13E-05	7.13E-05	7.13E-05	7.13E-05
SE 79	1.47E-04	1.47E-04	1.47E-04	1.47E-04	1.47E-04	1.47E-04	1.47E-04
SE 80	4.40E-04	4.40E-04	4.40E-04	4.40E-04	4.40E-04	4.40E-04	4.40E-04
BR 81	6.52E-04	6.52E-04	6.52E-04	6.52E-04	6.52E-04	6.52E-04	6.52E-04
SE 82	1.12E-03	1.12E-03	1.12E-03	1.12E-03	1.12E-03	1.12E-03	1.12E-03
KR 83	1.86E-03	1.86E-03	1.86E-03	1.86E-03	1.86E-03	1.86E-03	1.86E-03
KR 84	3.76E-03	3.77E-03	3.77E-03	3.77E-03	3.77E-03	3.77E-03	3.77E-03
KR 85	8.23E-04	8.24E-04	8.24E-04	8.24E-04	8.25E-04	8.25E-04	8.25E-04
RB 85	3.57E-03	3.57E-03	3.58E-03	3.58E-03	3.58E-03	3.58E-03	3.58E-03
KR 86	7.10E-03	7.10E-03	7.10E-03	7.10E-03	7.10E-03	7.10E-03	7.10E-03
RB 87	9.29E-03	9.29E-03	9.29E-03	9.29E-03	9.29E-03	9.29E-03	9.29E-03
SR 88	1.34E-02	1.34E-02	1.34E-02	1.34E-02	1.34E-02	1.34E-02	1.34E-02
SR 89	9.30E-04	9.32E-04	9.30E-04	9.28E-04	9.26E-04	9.23E-04	9.21E-04
Y 89	1.73E-02	1.73E-02	1.73E-02	1.73E-02	1.73E-02	1.73E-02	1.73E-02
SR 90	2.11E-02	2.11E-02	2.11E-02	2.11E-02	2.11E-02	2.11E-02	2.11E-02
Y 90	5.46E-06	5.46E-06	5.46E-06	5.46E-06	5.46E-06	5.46E-06	5.46E-06
ZR 90	1.16E-03	1.16E-03	1.16E-03	1.16E-03	1.16E-03	1.16E-03	1.16E-03
SR 91	7.02E-05	5.27E-05	3.94E-05	2.94E-05	2.20E-05	1.64E-05	1.23E-05
Y 91	1.26E-03	1.28E-03	1.29E-03	1.30E-03	1.30E-03	1.31E-03	1.31E-03
Y 91M	3.01E-06	2.88E-06	2.18E-06	1.63E-06	1.22E-06	9.09E-07	6.79E-07
ZR 91	2.13E-02	2.13E-02	2.13E-02	2.13E-02	2.13E-02	2.13E-02	2.13E-02
Y 92	2.89E-05	3.06E-05	2.02E-05	1.15E-05	6.05E-06	3.05E-06	1.50E-06
ZR 92	2.30E-02	2.30E-02	2.30E-02	2.30E-02	2.30E-02	2.30E-02	2.30E-02
Y 93	5.09E-05	4.00E-05	3.04E-05	2.31E-05	1.75E-05	1.33E-05	1.01E-05
ZR 93	1.64E-02	1.64E-02	1.64E-02	1.64E-02	1.64E-02	1.64E-02	1.65E-02
ZR 94	2.54E-02	2.54E-02	2.54E-02	2.54E-02	2.54E-02	2.54E-02	2.54E-02
ZR 95	1.65E-03	1.65E-03	1.65E-03	1.65E-03	1.64E-03	1.64E-03	1.64E-03
NB 95	8.52E-04	8.52E-04	8.53E-04	8.53E-04	8.53E-04	8.53E-04	8.53E-04
NB 95M	1.00E-06	1.00E-06	1.01E-06	1.01E-06	1.01E-06	1.01E-06	1.01E-06
MO 95	2.34E-02	2.34E-02	2.34E-02	2.34E-02	2.34E-02	2.34E-02	2.34E-02
ZR 96	2.52E-02	2.52E-02	2.52E-02	2.52E-02	2.52E-02	2.52E-02	2.52E-02
MO 96	9.63E-06	9.63E-06	9.63E-06	9.63E-06	9.63E-06	9.63E-06	9.64E-06
ZR 97	8.39E-05	7.12E-05	6.05E-05	5.13E-05	4.35E-05	3.70E-05	3.14E-05
NB 97	4.71E-06	5.26E-06	4.59E-06	3.91E-06	3.32E-06	2.82E-06	2.39E-06
MO 97	2.29E-02	2.29E-02	2.29E-02	2.29E-02	2.29E-02	2.29E-02	2.29E-02
MO 98	2.38E-02	2.38E-02	2.38E-02	2.38E-02	2.38E-02	2.38E-02	2.38E-02
MO 99	1.49E-04	1.43E-04	1.37E-04	1.31E-04	1.26E-04	1.21E-04	1.16E-04
TC 99	2.52E-02	2.52E-02	2.52E-02	2.52E-02	2.52E-02	2.52E-02	2.52E-02

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	INITIAL	0.2 D	0.3 D	0.5 D	0.7 D	0.8 D	1.0 D
TC 99M	7.16E-06	8.83E-06	9.71E-06	1.01E-05	1.02E-05	1.01E-05	9.84E-06
RU 99	1.00E-06	1.00E-06	1.00E-06	1.00E-06	1.00E-06	1.00E-06	1.00E-06
MO100	2.62E-02	2.62E-02	2.62E-02	2.62E-02	2.62E-02	2.62E-02	2.62E-02
RU100	1.24E-05	1.24E-05	1.24E-05	1.24E-05	1.24E-05	1.24E-05	1.24E-05
RU101	2.15E-02	2.15E-02	2.15E-02	2.15E-02	2.15E-02	2.15E-02	2.15E-02
RU102	1.81E-02	1.81E-02	1.81E-02	1.81E-02	1.81E-02	1.81E-02	1.81E-02
RU103	5.35E-04	5.34E-04	5.32E-04	5.31E-04	5.29E-04	5.28E-04	5.26E-04
RH103	1.26E-02	1.26E-02	1.26E-02	1.26E-02	1.26E-02	1.26E-02	1.26E-02
RU104	8.04E-03	8.05E-03	8.05E-03	8.05E-03	8.05E-03	8.05E-03	8.05E-03
PD104	4.73E-05	4.73E-05	4.73E-05	4.73E-05	4.73E-05	4.73E-05	4.73E-05
RH105	1.09E-05	1.47E-05	1.61E-05	1.63E-05	1.57E-05	1.49E-05	1.40E-05
PD105	4.29E-03	4.30E-03	4.30E-03	4.30E-03	4.30E-03	4.30E-03	4.30E-03
RU106	6.05E-04	6.05E-04	6.05E-04	6.05E-04	6.04E-04	6.04E-04	6.04E-04
PD106	1.23E-03	1.23E-03	1.23E-03	1.23E-03	1.23E-03	1.23E-03	1.23E-03
PD107	6.56E-04	6.57E-04	6.57E-04	6.57E-04	6.57E-04	6.57E-04	6.57E-04
PD108	3.19E-04	3.19E-04	3.19E-04	3.19E-04	3.19E-04	3.19E-04	3.19E-04
AG109	1.68E-04	1.68E-04	1.68E-04	1.68E-04	1.68E-04	1.68E-04	1.68E-04
PD110	1.44E-04	1.44E-04	1.44E-04	1.44E-04	1.44E-04	1.44E-04	1.44E-04
AG111	9.66E-07	9.86E-07	9.73E-07	9.59E-07	9.44E-07	9.30E-07	9.16E-07
CD111	9.41E-05	9.42E-05	9.42E-05	9.42E-05	9.42E-05	9.42E-05	9.42E-05
CD112	7.61E-05	7.62E-05	7.62E-05	7.62E-05	7.62E-05	7.63E-05	7.63E-05
CD113	3.02E-05	3.03E-05	3.04E-05	3.04E-05	3.04E-05	3.04E-05	3.04E-05
CD113M	1.15E-06	1.15E-06	1.15E-06	1.15E-06	1.15E-06	1.15E-06	1.15E-06
CD114	1.14E-04	1.14E-04	1.14E-04	1.14E-04	1.14E-04	1.14E-04	1.14E-04
IN115	5.08E-05	5.08E-05	5.08E-05	5.08E-05	5.09E-05	5.09E-05	5.09E-05
SN115	2.57E-06	2.58E-06	2.58E-06	2.58E-06	2.58E-06	8.28E-05	8.28E-05
SN117	5.35E-05	5.36E-05	5.36E-05	5.36E-05	5.36E-05	5.36E-05	5.36E-05
SN118	5.45E-05	5.46E-05	5.46E-05	5.46E-05	5.46E-05	5.46E-05	5.46E-05
SN119	6.10E-05	6.10E-05	6.10E-05	6.10E-05	6.10E-05	6.10E-05	6.10E-05
SN120	6.13E-05	6.13E-05	6.13E-05	6.13E-05	6.13E-05	6.13E-05	6.13E-05
SB121	6.56E-05	6.56E-05	6.56E-05	6.56E-05	6.57E-05	6.57E-05	6.57E-05
SN122	7.89E-05	7.89E-05	7.89E-05	7.89E-05	7.89E-05	7.89E-05	7.89E-05
SN123	1.12E-06	1.12E-06	1.11E-06	1.11E-06	1.11E-06	1.11E-06	1.11E-06
SB123	8.11E-05	8.12E-05	8.12E-05	8.12E-05	8.12E-05	8.12E-05	8.12E-05
SN124	1.35E-04	1.35E-04	1.35E-04	1.35E-04	1.35E-04	1.35E-04	1.35E-04
SB125	9.40E-05	9.40E-05	9.40E-05	9.40E-05	9.40E-05	9.40E-05	9.40E-05
TE125	5.89E-05	5.89E-05	5.89E-05	5.89E-05	5.89E-05	5.89E-05	5.90E-05
TE125M	1.21E-06	1.21E-06	1.21E-06	1.21E-06	1.21E-06	1.21E-06	1.21E-06
SN126	2.31E-04	2.31E-04	2.31E-04	2.31E-04	2.31E-04	2.31E-04	2.31E-04
TE126	1.37E-06	1.37E-06	1.37E-06	1.37E-06	1.37E-06	1.37E-06	1.37E-06
SB127	4.27E-06	4.44E-06	4.38E-06	4.27E-06	4.15E-06	4.03E-06	3.91E-06
TE127M	1.18E-05	1.18E-05	1.18E-05	1.18E-05	1.18E-05	1.18E-05	1.18E-05
I127	6.48E-04	6.48E-04	6.48E-04	6.48E-04	6.49E-04	6.49E-04	6.49E-04
TE128	1.89E-03	1.89E-03	1.89E-03	1.89E-03	1.89E-03	1.89E-03	1.89E-03
TE129M	2.47E-05	2.55E-05	2.58E-05	2.59E-05	2.60E-05	2.59E-05	2.59E-05
I129	4.03E-03	4.03E-03	4.04E-03	4.04E-03	4.04E-03	4.04E-03	4.04E-03
TE130	9.59E-03	9.59E-03	9.59E-03	9.59E-03	9.59E-03	9.59E-03	9.59E-03
XE130	3.60E-06	3.61E-06	3.61E-06	3.61E-06	3.62E-06	3.62E-06	3.62E-06
TE131M	8.85E-06	8.36E-06	7.62E-06	6.95E-06	6.34E-06	5.78E-06	5.27E-06

	INITIAL	0.2 D	0.3 D	0.5 D	0.7 D	0.8 D	1.0 D
I131	1.59E-04	1.86E-04	1.84E-04	1.82E-04	1.80E-04	1.78E-04	1.76E-04
XE131	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02	1.57E-02
XE131M	1.72E-06	1.73E-06	1.74E-06	1.75E-06	1.76E-06	1.77E-06	1.79E-06
TE132	1.51E-04	1.46E-04	1.41E-04	1.36E-04	1.32E-04	1.27E-04	1.23E-04
I132	3.53E-06	4.10E-06	4.16E-06	4.07E-06	3.95E-06	3.82E-06	3.69E-06
XE132	2.37E-02	2.37E-02	2.37E-02	2.37E-02	2.37E-02	2.37E-02	2.37E-02
I133	1.31E-04	1.30E-04	1.15E-04	1.00E-04	8.78E-05	7.69E-05	6.73E-05
XE133	1.95E-04	2.08E-04	2.19E-04	2.29E-04	2.36E-04	2.41E-04	2.46E-04
XE133M	2.56E-06	2.94E-06	3.24E-06	3.48E-06	3.65E-06	3.77E-06	3.84E-06
CS133	3.70E-02	3.70E-02	3.70E-02	3.70E-02	3.70E-02	3.70E-02	3.70E-02
XE134	4.39E-02	4.40E-02	4.40E-02	4.40E-02	4.40E-02	4.40E-02	4.40E-02
CS134	2.16E-05	2.16E-05	2.16E-05	2.16E-05	2.16E-05	2.16E-05	2.16E-05
BA134	1.11E-05	1.11E-05	1.11E-05	1.11E-05	1.11E-05	1.11E-05	1.11E-05
I135	9.84E-05	6.46E-05	4.23E-05	2.78E-05	1.82E-05	1.19E-05	7.83E-06
XE135	3.44E-05	5.46E-05	5.94E-05	5.63E-05	4.98E-05	4.21E-05	3.46E-05
CS135	3.51E-02	3.51E-02	3.51E-02	3.51E-02	3.51E-02	3.51E-02	3.51E-02
XE136	3.77E-02	3.77E-02	3.77E-02	3.77E-02	3.77E-02	3.77E-02	3.77E-02
CS136	7.33E-07	7.27E-07	7.21E-07	7.14E-07	7.08E-07	7.02E-07	6.96E-07
BA136	3.81E-05	3.81E-05	3.81E-05	3.81E-05	3.81E-05	3.81E-05	3.81E-05
CS137	3.43E-02	3.43E-02	3.43E-02	3.43E-02	3.43E-02	3.43E-02	3.43E-02
BA137	1.77E-03	1.77E-03	1.77E-03	1.77E-03	1.77E-03	1.77E-03	1.77E-03
BA138	3.88E-02	3.88E-02	3.88E-02	3.88E-02	3.88E-02	3.88E-02	3.88E-02
LA139	3.70E-02	3.70E-02	3.70E-02	3.70E-02	3.70E-02	3.70E-02	3.70E-02
BA140	5.71E-04	5.67E-04	5.62E-04	5.56E-04	5.51E-04	5.46E-04	5.42E-04
LA140	6.00E-05	6.10E-05	6.19E-05	6.26E-05	6.33E-05	6.39E-05	6.44E-05
CE140	3.73E-02	3.73E-02	3.73E-02	3.73E-02	3.73E-02	3.73E-02	3.73E-02
LA141	7.34E-05	4.10E-05	2.02E-05	9.96E-06	4.91E-06	2.42E-06	1.19E-06
CE141	1.09E-03	1.13E-03	1.15E-03	1.16E-03	1.16E-03	1.15E-03	1.15E-03
PR141	3.31E-02	3.31E-02	3.31E-02	3.31E-02	3.31E-02	3.31E-02	3.31E-02
CE142	3.49E-02	3.50E-02	3.50E-02	3.50E-02	3.50E-02	3.50E-02	3.50E-02
ND142	8.19E-06	8.20E-06	8.20E-06	8.21E-06	8.22E-06	8.22E-06	8.23E-06
CE143	1.53E-04	1.48E-04	1.36E-04	1.25E-04	1.15E-04	1.06E-04	9.70E-05
PR143	4.55E-04	4.64E-04	4.72E-04	4.79E-04	4.85E-04	4.90E-04	4.94E-04
ND143	3.48E-02	3.48E-02	3.48E-02	3.48E-02	3.48E-02	3.48E-02	3.48E-02
CE144	8.69E-03	8.68E-03	8.68E-03	8.68E-03	8.67E-03	8.67E-03	8.67E-03
ND144	2.46E-02	2.46E-02	2.46E-02	2.46E-02	2.46E-02	2.46E-02	2.46E-02
PR145	6.28E-05	4.03E-05	2.53E-05	1.59E-05	1.00E-05	6.31E-06	3.97E-06
ND145	2.37E-02	2.38E-02	2.38E-02	2.38E-02	2.38E-02	2.38E-02	2.38E-02
ND146	1.82E-02	1.82E-02	1.82E-02	1.82E-02	1.82E-02	1.82E-02	1.82E-02
ND147	1.89E-04	1.90E-04	1.88E-04	1.86E-04	1.84E-04	1.82E-04	1.80E-04
PM147	8.20E-03	8.20E-03	8.20E-03	8.20E-03	8.20E-03	8.20E-03	8.20E-03
SM147	5.46E-03	5.46E-03	5.47E-03	5.47E-03	5.47E-03	5.47E-03	5.47E-03
ND148	1.04E-02	1.04E-02	1.04E-02	1.04E-02	1.04E-02	1.04E-02	1.04E-02
PM148M	1.32E-06	1.31E-06	1.31E-06	1.31E-06	1.30E-06	1.30E-06	1.30E-06
SM148	4.41E-05	4.41E-05	4.41E-05	4.41E-05	4.41E-05	4.41E-05	4.41E-05
PM149	2.76E-05	3.32E-05	3.29E-05	3.15E-05	3.00E-05	2.85E-05	2.70E-05
SM149	1.66E-03	1.67E-03	1.67E-03	1.67E-03	1.67E-03	1.67E-03	1.67E-03
ND150	4.09E-03	4.09E-03	4.09E-03	4.09E-03	4.09E-03	4.09E-03	4.09E-03
SM150	5.00E-03	5.00E-03	5.00E-03	5.00E-03	5.00E-03	5.00E-03	5.00E-03
PM151	1.10E-05	1.04E-05	9.41E-06	8.53E-06	7.74E-06	7.02E-06	6.36E-06

	INITIAL	0.2 D	0.3 D	0.5 D	0.7 D	0.8 D	1.0 D
SM151	2.19E-03	2.19E-03	2.19E-03	2.19E-03	2.19E-03	2.19E-03	2.19E-03
EU151	3.54E-05	3.54E-05	3.54E-05	3.54E-05	3.55E-05	3.55E-05	3.55E-05
SM152	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03	2.13E-03
EU152	2.64E-06	2.64E-06	2.64E-06	2.64E-06	2.64E-06	2.64E-06	2.64E-06
GD152	1.16E-06	1.16E-06	1.16E-06	1.16E-06	1.16E-06	1.16E-06	1.16E-06
SM153	5.30E-06	5.08E-06	4.79E-06	4.51E-06	4.24E-06	4.00E-06	3.77E-06
EU153	1.04E-03	1.04E-03	1.04E-03	1.04E-03	1.04E-03	1.04E-03	1.04E-03
SM154	4.77E-04	4.78E-04	4.78E-04	4.78E-04	4.78E-04	4.78E-04	4.78E-04
EU154	7.89E-06	7.89E-06	7.89E-06	7.89E-06	7.89E-06	7.89E-06	7.89E-06
GD154	9.07E-07	9.07E-07	9.08E-07	9.08E-07	9.08E-07	9.09E-07	9.09E-07
EU155	1.44E-04	1.44E-04	1.44E-04	1.44E-04	1.44E-04	1.44E-04	1.44E-04
GD155	3.21E-05	3.21E-05	3.21E-05	3.21E-05	3.21E-05	3.22E-05	3.22E-05
EU156	1.78E-06	1.84E-06	1.87E-06	1.90E-06	1.91E-06	1.92E-06	1.92E-06
GD156	1.20E-04	1.20E-04	1.20E-04	1.20E-04	1.21E-04	1.21E-04	1.21E-04
GD157	6.41E-06	6.44E-06	6.46E-06	6.47E-06	6.49E-06	6.50E-06	6.51E-06
GD158	5.50E-05	5.50E-05	5.50E-05	5.50E-05	5.50E-05	5.50E-05	5.50E-05
TB159	6.91E-06	6.91E-06	6.91E-06	6.92E-06	6.92E-06	6.92E-06	6.92E-06
GD160	2.23E-06	2.23E-06	2.23E-06	2.23E-06	2.23E-06	2.23E-06	2.23E-06
TOTAL	9.71E-01	9.71E-01	9.71E-01	9.71E-01	9.71E-01	9.71E-01	9.71E-01

Appendix E: Model Comparison Data

Table E-1: Model Comparison Nuclide Concentrations

Isotope	Model 1	Model 2	Model 3	Model 4	Model 5	Model 6
			Concentration (g)			
HE-4	1.31E-06	9.24E-06	8.98E-06	1.69E-06	6.28E-06	6.12E-06
TH230	6.62E-06	6.62E-06	6.62E-06	4.14E-06	4.14E-06	4.14E-06
U-234	2.97E-01	2.97E-01	2.97E-01	1.86E-01	1.86E-01	1.86E-01
U-235	3.79	3.79	3.79	2.37	2.37	2.37
U-236	0.171	0.171	0.171	0.108	0.108	0.108
U-237	3.24E-05	3.24E-05	3.24E-05	2.04E-05	2.04E-05	2.04E-05
U-238	1.61E+02	1.61E+02	1.61E+02	1.01E+02	1.01E+02	1.01E+02
NP-237	1.25E-04	1.26E-04	1.26E-04	7.96E-05	7.91E-05	7.91E-05
NP-239	4.89E-03	4.90E-03	4.90E-03	3.08E-03	3.08E-03	3.08E-03
PU-239	4.90E-02	4.92E-02	4.92E-02	3.11E-02	3.09E-02	3.09E-02
PU-240	3.83E-04	3.85E-04	3.84E-04	2.45E-04	2.43E-04	2.43E-04

Appendix F: Power History Comparison Data

Table F-1: Power History Comparison Nuclide Concentrations

Nuclide	History 1	History 2	History 3	History 4	History 5	History 6	History 7
				Concentration (g)			
HE-4	9.24E-06	8.99E-06	5.42E-05	9.24E-06	8.99E-06	2.77E-06	9.23E-06
CR-57	0.00E+00	3.88E-06	2.71E-06	0.00E+00	3.55E-06	9.36E-07	5.25E-06
FE-56	0.00E+00	0.00E+00	3.87E-06	0.00E+00	0.00E+00	0.00E+00	0.00E+00
NI-63	0.00E+00	0.00E+00	7.20E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00
SR-89	9.40E-05	7.75E-04	4.59E-04	9.20E-05	7.38E-04	2.93E-04	9.30E-04
Y-91	9.41E-05	1.07E-03	6.12E-04	9.11E-05	1.02E-03	4.25E-04	1.26E-03
Y-91M	2.71E-06	2.70E-06	0.00E+00	2.71E-06	2.70E-06	2.70E-06	3.01E-06
ZR-95	2.22E-04	1.41E-03	8.06E-04	2.16E-04	1.36E-03	6.60E-04	1.65E-03
NB-95	1.55E-04	8.18E-04	3.97E-04	1.53E-04	8.14E-04	5.55E-04	8.52E-04
MO-96	8.82E-06	9.07E-06	1.04E-05	8.79E-06	9.05E-06	9.48E-06	9.63E-06
NB-95M	0.00E+00	8.79E-07	0.00E+00	0.00E+00	0.00E+00	0.00E+00	0.00E+00
RU-103	5.22E-05	4.28E-04	2.74E-04	5.17E-05	4.01E-04	1.29E-04	5.35E-04
RU-106	4.31E-04	5.17E-04	3.05E-04	4.27E-04	5.13E-04	5.20E-04	6.05E-04
SN-123	0.00E+00	9.58E-07	0.00E+00	0.00E+00	0.00E+00	7.15E-07	1.12E-06
TE-125	7.01E-05	6.65E-05	9.27E-05	7.04E-05	6.68E-05	6.41E-05	5.89E-05
TE-127M	3.32E-06	1.06E-05	5.53E-06	3.23E-06	1.04E-05	7.10E-06	1.18E-05
TE-129M	1.08E-06	1.88E-05	1.27E-05	1.07E-06	1.74E-05	3.77E-06	2.47E-05
I-131	3.96E-05	7.60E-05	9.55E-05	3.96E-05	6.71E-05	3.96E-05	1.59E-04
TE-132	8.12E-05	8.41E-05	1.03E-04	8.12E-05	8.31E-05	8.11E-05	1.51E-04
XE-133	9.36E-06	4.37E-05	1.16E-04	9.36E-06	3.39E-05	9.34E-06	1.95E-04
BA-134	1.22E-05	1.08E-05	1.80E-05	1.14E-05	1.02E-05	1.17E-05	1.11E-05
CS-135	1.91E-02	2.14E-02	1.51E-05	1.53E-05	1.83E-05	1.90E-05	2.16E-05
XE-136	5.38E-02	5.15E-02	3.68E-02	5.94E-02	5.50E-02	4.50E-02	3.77E-02
BA-137	2.15E-03	2.06E-03	3.50E-03	2.16E-03	2.07E-03	1.94E-03	1.77E-03
BA-140	1.30E-04	3.36E-04	3.23E-04	1.30E-04	2.97E-04	1.30E-04	5.71E-04
LA-140	1.01E-06	3.23E-05	2.99E-05	1.01E-06	2.64E-05	1.08E-06	6.00E-05
CE-141	4.52E-05	8.29E-04	5.64E-04	4.48E-05	7.62E-04	1.55E-04	1.09E-03
ND-142	6.83E-06	7.17E-06	8.53E-06	6.69E-06	7.06E-06	7.76E-06	4.55E-04
PR-143	6.80E-06	2.53E-04	2.29E-04	6.80E-06	2.09E-04	7.65E-06	4.55E-04
CE-144	5.56E-03	7.31E-03	4.23E-03	5.50E-03	7.25E-03	7.13E-03	8.69E-03
ND-147	4.61E-05	1.05E-04	1.09E-04	4.61E-05	9.29E-05	4.61E-05	1.89E-04
SM-147	6.57E-03	6.21E-03	8.47E-03	6.61E-03	6.25E-03	6.00E-03	5.46E-03
SM-148	3.62E-05	3.70E-05	4.02E-05	3.42E-05	3.55E-05	4.15E-05	4.41E-05
SM-149	1.92E-03	1.79E-03	1.67E-03	2.08E-03	1.86E-03	1.76E-03	1.66E-03
EU-154	7.13E-06	7.37E-06	7.07E-06	6.63E-06	7.16E-06	7.57E-06	7.89E-06
GD-154	1.13E-06	1.01E-06	1.79E-06	1.08E-06	9.65E-07	1.02E-06	9.07E-07
GD-155	4.29E-05	3.78E-05	5.53E-05	4.32E-05	3.80E-05	3.68E-05	3.21E-05
EU-156	0.00E+00	1.01E-06	9.15E-07	0.00E+00	8.68E-07	0.00E+00	1.78E-06

Nuclide	History 1	History 2	History 3	History 4	History 5	History 6	History 7
			Concentration (g)				
U-235	3.79E+01	3.79E+01	3.79E+01	3.79E+01	3.79E+01	3.79E+01	3.79E+01
U-238	1.61E+02	1.61E+02	1.61E+02	1.61E+02	1.61E+02	1.61E+02	1.61E+02
U-237	0	1.05E-06	1.28E-06	0	9.65E-07	0	2.06E-06
PU-239	5.39E-02	5.39E-02	5.69E-02	5.40E-02	5.39E-02	5.32E-02	5.36E-02
PU-240	3.99E-04	4.04E-04	4.65E-04	3.85E-04	3.94E-04	4.06E-04	4.22E-04

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Vita

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13. ABSTRACT *(Maximum 200 words)*

The purpose of this study was to develop a methodology for creating problem-dependent cross section libraries for ORIGEN (Oak Ridge Isotope Generation and Depletion Code). The Air Force Technical Applications Center (AFTAC) has a requirement to classify spent nuclear fuel. The ORIGEN codes provide generic models of commercial nuclear reactor designs that are not adequate for the detailed analysis required by AFTAC. After comparing the methods that ORIGEN2 and ORIGEN-S use to develop burnup-dependent cross section libraries, the research focused on developing a methodology for creating new ORIGEN-S models. Models of the Ohio State University Research Reactor were created using the Coupled 1-D Shielding Analysis (SAS2H) module of the Modular Code System for Performing Standardized Computer Analysis for Licensing Evaluation (SCALE4.3). Model design parameters were examined by varying the fuel loading, composition temperatures, larger unit cells, and power histories. The results indicate that the SAS2H sequence has the potential to fulfill the technical requirements of the sponsor.

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